trans-1,2-ethylmethylcyclopentane

Other names: 1-Ethyl-2-methylcyclopentane, (Z)-
1-Ethyl-2-methylcyclopentane, cis
1-Methyl-cis-2-ethylcyclopentane
c-1-Ethyl-2-methylcyclopentane
cis-1-Ethyl-2-Methylcyclopentane
cis-1-Methyl-2-ethylcyclopentane
Inchi: InChI=1S/C8H16/c1-3-8-6-4-5-7(8)2/h7-8H,3-6H2,1-2H3/t7-,8+/m0/s1
InchiKey: BSKOLJVTLRLTHE-JGVFFNPUSA-N
Formula: C8H16
SMILES: CCC1CCCC1C
Mol. weight [g/mol]: 112.21
CAS: 930-89-2

Physical Properties

Property code	Value	Unit	Source
af	0.2625		Cheméo Relay (1.0)
chl	-5243.89 ± 0.92	kJ/mol	NIST Webbook
gf	45.32	kJ/mol	Joback Method
hf	-149.95	kJ/mol	Cheméo Relay (1.0)
hfl	-190.80 ± 1.00	kJ/mol	NIST Webbook
hfus	11.48	kJ/mol	Joback Method
hvap	40.20	kJ/mol	NIST Webbook
ie	9.27	eV	Cheméo Relay (1.0)
log10ws	-4.56		Cheméo Relay (1.0)
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	822.00		NIST Webbook
rinpol	829.80		NIST Webbook
rinpol	825.40		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	828.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	823.00		NIST Webbook

rinpol	824.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	829.00	NIST Webbook
rinpol	821.10	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	846.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	830.00	NIST Webbook
rinpol	837.00	NIST Webbook
rinpol	820.60	NIST Webbook
rinpol	815.95	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	818.90	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	832.00	NIST Webbook
rinpol	817.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	820.80	NIST Webbook
rinpol	821.30	NIST Webbook
rinpol	823.20	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	828.10	NIST Webbook
rinpol	825.30	NIST Webbook
rinpol	831.30	NIST Webbook
rinpol	820.00	NIST Webbook
rinpol	822.00	NIST Webbook
rinpol	825.00	NIST Webbook
rinpol	827.00	NIST Webbook
rinpol	829.00	NIST Webbook
rinpol	831.00	NIST Webbook
rinpol	820.10	NIST Webbook
rinpol	825.30	NIST Webbook
rinpol	821.00	NIST Webbook
rinpol	826.00	NIST Webbook
rinpol	816.00	NIST Webbook
rinpol	820.60	NIST Webbook
rinpol	790.00	NIST Webbook
rinpol	828.10	NIST Webbook
rinpol	825.00	NIST Webbook

rinpol	787.51		NIST Webbook
rinpol	820.10		NIST Webbook
rinpol	825.30		NIST Webbook
rinpol	820.70		NIST Webbook
rinpol	820.30		NIST Webbook
tb	401.20 ± 0.30	K	NIST Webbook
tb	401.20 ± 0.02	K	NIST Webbook
tb	401.00 ± 2.00	K	NIST Webbook
tb	401.20 ± 0.20	K	NIST Webbook
tb	401.20	K	KDB
tb	401.20	K	NIST Webbook
tb	401.10 ± 0.10	K	NIST Webbook
tc	591.87	K	Cheméo Relay (1.0)
tf	167.14 ± 0.10	K	NIST Webbook
tf	379.10 ± 0.10	K	NIST Webbook
tf	164.40 ± 3.00	K	NIST Webbook
tf	167.20 ± 0.07	K	NIST Webbook
tf	167.21 ± 0.06	K	NIST Webbook
tf	164.40 ± 2.00	K	NIST Webbook
tf	166.46 ± 0.06	K	NIST Webbook
tf	166.45 ± 0.30	K	NIST Webbook
vc	0.399	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.17	J/mol×K	521.15	Joback Method
cpg	303.19	J/mol×K	585.20	Joback Method
cpg	290.01	J/mol×K	553.18	Joback Method
cpg	261.64	J/mol×K	489.13	Joback Method
cpg	213.75	J/mol×K	393.05	Joback Method
cpg	230.45	J/mol×K	425.08	Joback Method
cpg	246.41	J/mol×K	457.10	Joback Method
dvisc	0.0022106	Pa×s	186.58	Joback Method
dvisc	0.0012051	Pa×s	220.99	Joback Method
dvisc	0.0007737	Pa×s	255.40	Joback Method
dvisc	0.0005518	Pa×s	289.81	Joback Method
dvisc	0.0004228	Pa×s	324.23	Joback Method
dvisc	0.0003410	Pa×s	358.64	Joback Method
dvisc	0.0002855	Pa×s	393.05	Joback Method
hvapt	38.30	kJ/mol	362.00	NIST Webbook

hvapt	39.30	kJ/mol	353.00	NIST Webbook
hvapt	42.50	kJ/mol	271.00	NIST Webbook
hvapt	41.60	kJ/mol	263.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39419e+01
Coeff. B	-3.21987e+03
Coeff. C	-5.57510e+01
Temperature range (K), min.	291.57
Temperature range (K), max.	428.84

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.66373e+01
Coeff. B	-7.06332e+03
Coeff. C	-9.36311e+00
Coeff. D	1.22005e-05
Temperature range (K), min.	238.15
Temperature range (K), max.	288.15

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C930892&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=483

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=483

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume