Cyclopentane, 1-ethyl-3-methyl-

Other names: 1-Ethyl-3-methylcyclopentane
1-Methyl-3-ethylcyclopentane
Inchi: InChI=1S/C8H16/c1-3-8-5-4-7(2)6-8/h7-8H,3-6H2,1-2H3
InchiKey: PQXAPVOKLYINEI-UHFFFAOYSA-N
Formula: C8H16
SMILES: CCC1CCC(C)C1
Mol. weight [g/mol]: 112.21
CAS: 3726-47-4

Physical Properties

Property code	Value	Unit	Source
gf	45.32	kJ/mol	Joback Method
hf	-168.31	kJ/mol	Joback Method
hfus	11.48	kJ/mol	Joback Method
hvap	33.35	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	785.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	793.90		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	793.90		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	792.00		NIST Webbook
rinpol	785.00		NIST Webbook
tb	394.24 ± 0.70	K	NIST Webbook
tb	394.18 ± 0.20	K	NIST Webbook
tc	585.20	K	Joback Method
tf	145.13 ± 0.15	K	NIST Webbook
tf	140.40 ± 1.00	K	NIST Webbook
tf	140.35 ± 2.00	K	NIST Webbook
tf	140.50 ± 0.50	K	NIST Webbook

vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	261.64	J/mol×K	489.13	Joback Method
cpg	276.17	J/mol×K	521.15	Joback Method
cpg	290.01	J/mol×K	553.18	Joback Method
cpg	303.19	J/mol×K	585.20	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35282e+01
Coeff. B	-3.06019e+03
Coeff. C	-5.07380e+01
Temperature range (K), min.	281.86
Temperature range (K), max.	423.17

Sources

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

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3726474&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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