Cyclohexene, 3-ethyl-

Other names: 3-Ethyl-1-cyclohexene
3-Ethylcyclohexene
Inchi: InChI=1S/C8H14/c1-2-8-6-4-3-5-7-8/h4,6,8H,2-3,5,7H2,1H3
InchiKey: BAGSBIKCNLYDJO-UHFFFAOYSA-N
Formula: C8H14
SMILES: CCC1C=CCCC1
Mol. weight [g/mol]: 110.20
CAS: 2808-71-1

Physical Properties

Property code	Value	Unit	Source
gf	70.89	kJ/mol	Joback Method
hf	-96.35	kJ/mol	Joback Method
hfus	9.53	kJ/mol	Joback Method
hvap	34.12	kJ/mol	Joback Method
ie	8.83 ± 0.01	eV	NIST Webbook
log10ws	-2.68		Crippen Method
logp	2.753		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpol	843.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	848.70		NIST Webbook
rinpol	843.00		NIST Webbook
rinpol	843.20		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	853.00		NIST Webbook
ripol	983.00		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	993.00		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	1004.10		NIST Webbook
ripol	983.20		NIST Webbook

ripol	993.30		NIST Webbook
ripol	1004.10		NIST Webbook
ripol	983.20		NIST Webbook
ripol	993.30		NIST Webbook
tb	405.00 ± 1.00	K	NIST Webbook
tc	604.14	K	Joback Method
tf	188.06	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.84	J/mol×K	401.15	Joback Method
cpg	216.08	J/mol×K	434.98	Joback Method
cpg	231.52	J/mol×K	468.81	Joback Method
cpg	246.17	J/mol×K	502.64	Joback Method
cpg	260.07	J/mol×K	536.48	Joback Method
cpg	273.23	J/mol×K	570.31	Joback Method
cpg	285.67	J/mol×K	604.14	Joback Method
dvisc	0.0057600	Pa×s	188.06	Joback Method
dvisc	0.0022895	Pa×s	223.57	Joback Method
dvisc	0.0011720	Pa×s	259.09	Joback Method
dvisc	0.0007050	Pa×s	294.61	Joback Method
dvisc	0.0004731	Pa×s	330.12	Joback Method
dvisc	0.0003431	Pa×s	365.63	Joback Method
dvisc	0.0002634	Pa×s	401.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39460e+01
Coeff. B	-3.22591e+03
Coeff. C	-5.91560e+01
Temperature range (K), min.	295.34
Temperature range (K), max.	432.76

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2808711&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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume