Cyclohexanol, 1-ethyl-

Other names: 1-Aethyl-cyclohexanol-(1)
1-Ethylcyclohexanol
Inchi: InChI=1S/C8H16O/c1-2-8(9)6-4-3-5-7-8/h9H,2-7H2,1H3
InchiKey: BUCJHJXFXUZJHL-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCC1(O)CCCCC1
Mol. weight [g/mol]: 128.21
CAS: 1940-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-101.38	kJ/mol	Joback Method
hf	-291.12	kJ/mol	Joback Method
hfus	6.10	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.092		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	439.20	K	NIST Webbook
tb	439.00 ± 6.00	K	NIST Webbook
tc	692.80	K	Joback Method
tf	272.02	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.97	J/mol×K	494.41	Joback Method
cpg	289.78	J/mol×K	527.48	Joback Method
cpg	303.67	J/mol×K	560.54	Joback Method
cpg	316.73	J/mol×K	593.61	Joback Method
cpg	329.04	J/mol×K	626.67	Joback Method
cpg	340.69	J/mol×K	659.74	Joback Method

cpg	351.77	J/mol×K	692.80	Joback Method
hvapt	46.90	kJ/mol	382.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61139e+01
Coeff. B	-4.32195e+03
Coeff. C	-6.32340e+01
Temperature range (K), min.	307.65
Temperature range (K), max.	463.32

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1940187&Units=SI

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

Legend

cpg: Ideal gas heat capacity
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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume