Cyclohexanol, 3,3-dimethyl-

Other names: 3,3-Dimethylcyclohexanol
Inchi: InChI=1S/C8H16O/c1-8(2)5-3-4-7(9)6-8/h7,9H,3-6H2,1-2H3
InchiKey: DQBDGNSFXSCBJX-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CC1(C)CCCC(O)C1
Mol. weight [g/mol]: 128.21
CAS: 767-12-4

Physical Properties

Property code	Value	Unit	Source
gf	-109.09	kJ/mol	Joback Method
hf	-311.46	kJ/mol	Joback Method
hfus	7.17	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.948		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	457.00 ± 2.00	K	NIST Webbook
tb	456.00 ± 2.00	K	NIST Webbook
tc	687.88	K	Joback Method
tf	284.70 ± 2.00	K	NIST Webbook
tf	284.00 ± 3.00	K	NIST Webbook
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.75	J/mol×K	489.74	Joback Method
cpg	290.94	J/mol×K	522.76	Joback Method
cpg	305.22	J/mol×K	555.79	Joback Method
cpg	318.68	J/mol×K	588.81	Joback Method

cpg	331.39	J/mol×K	621.83	Joback Method
cpg	343.44	J/mol×K	654.85	Joback Method
cpg	354.91	J/mol×K	687.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.63490e+01
Coeff. B	-4.54543e+03
Coeff. C	-6.85160e+01
Temperature range (K), min.	351.52
Temperature range (K), max.	480.33

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C767124&Units=SI

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
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