Cyclohexanol, 3,3,5-trimethyl-, cis-

Other names: 3,3,5-Trimethylcyclohexanol, (Z)-
cis-3,3,5-Trimethylcyclohexanol
cis-3,5,5-trimethylcyclohexan-1-ol
Inchi: InChI=1S/C9H18O/c1-7-4-8(10)6-9(2,3)5-7/h7-8,10H,4-6H2,1-3H3/t7-,8+/m1/s1
InchiKey: BRRVXFOKWJKTGG-SFYZADRCSA-N
Formula: C9H18O
SMILES: CC1CC(O)CC(C)(C)C1
Mol. weight [g/mol]: 142.24
CAS: 933-48-2

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-352.44	kJ/mol	Joback Method
hfus	10.83	kJ/mol	Joback Method
hvap	50.97	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.194		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	507.95	K	Joback Method
tc	703.29	K	Joback Method
tf	310.90 ± 2.00	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.20	J/mol×K	507.95	Joback Method
cpg	338.50	J/mol×K	540.51	Joback Method
cpg	353.91	J/mol×K	573.06	Joback Method
cpg	368.51	J/mol×K	605.62	Joback Method
cpg	382.36	J/mol×K	638.18	Joback Method
cpg	395.55	J/mol×K	670.73	Joback Method

cpg	408.14	J/mol×K	703.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53419e+01
Coeff. B	-4.39401e+03
Coeff. C	-7.32420e+01
Temperature range (K), min.	365.12
Temperature range (K), max.	511.31

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=C933482&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
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