Cyclohexanol, 3,3,5-trimethyl-, trans-

Other names:	3,3,5-Trimethylcyclohexanol, (E)- trans-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-HTQZYQBOSA-N
Formula:	C9H18O
SMILES:	CC1CC(O)CC(C)(C)C1
Mol. weight [g/mol]:	142.24
CAS:	767-54-4

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
rinpol	1119.00		NIST Webbook
rinpol	1119.00		NIST Webbook
tb	507.95	K	Joback Method
tc	703.29	K	Joback Method
tf	330.20 ± 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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C767544&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume