

3,3-dimethylcyclohexaneethanol

Inchi:	InChI=1S/C10H20O/c1-10(2)6-3-4-9(8-10)5-7-11/h9,11H,3-8H2,1-2H3
InchiKey:	SDCAHEIMKVRZEX-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CC1(C)CCCC(CCO)C1
Mol. weight [g/mol]:	156.27

Physical Properties

Property code	Value	Unit	Source
gf	-92.25	kJ/mol	Joback Method
hf	-352.74	kJ/mol	Joback Method
hfus	12.35	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.585		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1195.00		NIST Webbook
tb	535.50	K	Joback Method
tc	728.56	K	Joback Method
tf	290.32	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.93	J/mol×K	535.50	Joback Method
cpg	385.49	J/mol×K	567.68	Joback Method
cpg	401.15	J/mol×K	599.85	Joback Method
cpg	416.00	J/mol×K	632.03	Joback Method
cpg	430.10	J/mol×K	664.21	Joback Method
cpg	443.56	J/mol×K	696.38	Joback Method
cpg	456.43	J/mol×K	728.56	Joback Method

Sources

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=R216390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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