

(3,3-dimethyl-1-cyclohexyl)-1-methanol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C9H18O/c1-9(2)5-3-4-8(6-9)7-10/h8,10H,3-7H2,1-2H3

VJZDBRGSBDTGKQ-UHFFFAOYSA-N

C9H18O

CC1(C)CCCC(CO)C1

142.24

Physical Properties

Property code	Value	Unit	Source
gf	-100.67	kJ/mol	Joback Method
hf	-332.10	kJ/mol	Joback Method
hfus	9.76	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.195		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
ripol	1697.00		NIST Webbook
ripol	1697.00		NIST Webbook
tb	512.62	K	Joback Method
tc	708.19	K	Joback Method
tf	279.05	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.47	J/mol×K	512.62	Joback Method
cpg	337.38	J/mol×K	545.22	Joback Method
cpg	352.40	J/mol×K	577.81	Joback Method
cpg	366.59	J/mol×K	610.41	Joback Method
cpg	380.04	J/mol×K	643.00	Joback Method
cpg	392.82	J/mol×K	675.60	Joback Method
cpg	405.03	J/mol×K	708.19	Joback Method

Sources

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=R344113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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