

1-Cyclohexyl-2,2-dimethyl-1-propanol

Inchi:	InChI=1S/C11H22O/c1-11(2,3)10(12)9-7-5-4-6-8-9/h9-10,12H,4-8H2,1-3H3
InchiKey:	SHNBWIOMPFKTMH-UHFFFAOYSA-N
Formula:	C11H22O
SMILES:	CC(C)(C)C(O)C1CCCCC1
Mol. weight [g/mol]:	170.29
CAS:	62039-14-9

Physical Properties

Property code	Value	Unit	Source
gf	-70.23	kJ/mol	Joback Method
hf	-382.31	kJ/mol	Joback Method
hfus	9.23	kJ/mol	Joback Method
hvap	55.50	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.974		Crippen Method
mcvol	160.860	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	559.14	K	Joback Method
tc	757.69	K	Joback Method
tf	269.35	K	Joback Method
vc	0.587	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.42	J/molxK	559.14	Joback Method
cpg	502.98	J/molxK	724.59	Joback Method
cpg	488.62	J/molxK	691.50	Joback Method
cpg	473.33	J/molxK	658.41	Joback Method
cpg	457.06	J/molxK	625.32	Joback Method
cpg	439.77	J/molxK	592.23	Joback Method
cpg	516.46	J/molxK	757.69	Joback Method
dvisc	0.0000896	Paxs	559.14	Joback Method
dvisc	0.0001610	Paxs	510.84	Joback Method

dvisc	0.0003272	Paxs	462.54	Joback Method
dvisc	0.0007844	Paxs	414.25	Joback Method
dvisc	0.0023684	Paxs	365.95	Joback Method
dvisc	0.0100076	Paxs	317.65	Joback Method
dvisc	0.0709016	Paxs	269.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62039149&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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