

Cyclohexanemethanol, «alpha»-methyl-, (S)-

Inchi:	InChI=1S/C8H16O/c1-7(9)8-5-3-2-4-6-8/h7-9H,2-6H2,1H3/t7-/m1/s1
InchiKey:	JMSUNAQVHOHLMX-SSDOTTSWSA-N
Formula:	C8H16O
SMILES:	CC(O)C1CCCCC1
Mol. weight [g/mol]:	128.21
CAS:	3113-98-2

Physical Properties

Property code	Value	Unit	Source
gf	-98.33	kJ/mol	Joback Method
hf	-311.64	kJ/mol	Joback Method
hfus	8.88	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.948		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	493.73	K	Joback Method
tc	688.47	K	Joback Method
tf	233.12	K	Joback Method
vc	0.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.89	J/mol×K	493.73	Joback Method
cpg	290.13	J/mol×K	526.19	Joback Method
cpg	304.61	J/mol×K	558.64	Joback Method
cpg	318.34	J/mol×K	591.10	Joback Method
cpg	331.35	J/mol×K	623.56	Joback Method
cpg	343.66	J/mol×K	656.01	Joback Method
cpg	355.28	J/mol×K	688.47	Joback Method
dvisc	0.1298212	Paxs	233.12	Joback Method
dvisc	0.0178461	Paxs	276.56	Joback Method

dvisc	0.0042044	Paxs	319.99	Joback Method
dvisc	0.0013994	Paxs	363.42	Joback Method
dvisc	0.0005891	Paxs	406.86	Joback Method
dvisc	0.0002930	Paxs	450.29	Joback Method
dvisc	0.0001648	Paxs	493.73	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	4.70	NIST Webbook
tbrp	355.70	K	1.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3113982&Units=SI

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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