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	m3/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	Pa×s	233.12	Joback Method
dvisc	0.0178461	Pa×s	276.56	Joback Method

dvisc	0.0042044	Pa×s	319.99	Joback Method
dvisc	0.0013994	Pa×s	363.42	Joback Method
dvisc	0.0005891	Pa×s	406.86	Joback Method
dvisc	0.0002930	Pa×s	450.29	Joback Method
dvisc	0.0001648	Pa×s	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3113982&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
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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