Cyclooctyl alcohol

Other names: Cyclooctanol
Inchi: InChI=1S/C8H16O/c9-8-6-4-2-1-3-5-7-8/h8-9H,1-7H2
InchiKey: FHADSMKORVFYOS-UHFFFAOYSA-N
Formula: C8H16O
SMILES: OC1CCCCCCC1
Mol. weight [g/mol]: 128.21
CAS: 696-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-120.09	kJ/mol	Joback Method
hf	-318.68	kJ/mol	Joback Method
hfus	8.20	kJ/mol	Joback Method
hvap	50.85	kJ/mol	Joback Method
log10ws	-1.29		Aqueous Solubility Prediction Method
log10ws	-1.29		Estimated Solubility Method
logp	2.092		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1147.30		NIST Webbook
rinpol	1131.40		NIST Webbook
rinpol	1155.00		NIST Webbook
ripol	1640.80		NIST Webbook
ripol	1700.00		NIST Webbook
tb	502.71	K	Joback Method
tc	707.64	K	Joback Method
tf	291.52	K	Aqueous Solubility Prediction Method
tt	263.56	K	Heat capacities of selected cycloalcohols
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.72	J/mol×K	502.71	Joback Method
cpg	291.42	J/mol×K	536.87	Joback Method
cpg	307.29	J/mol×K	571.02	Joback Method
cpg	322.32	J/mol×K	605.18	Joback Method
cpg	336.54	J/mol×K	639.33	Joback Method
cpg	349.95	J/mol×K	673.49	Joback Method
cpg	362.56	J/mol×K	707.64	Joback Method
dvisc	0.0001108	Pa×s	502.71	Joback Method
dvisc	0.0178103	Pa×s	284.69	Joback Method
dvisc	0.0037588	Pa×s	328.29	Joback Method
dvisc	0.1481500	Pa×s	241.08	Joback Method
dvisc	0.0004459	Pa×s	415.50	Joback Method
dvisc	0.0002081	Pa×s	459.10	Joback Method
dvisc	0.0011425	Pa×s	371.89	Joback Method
hfust	2.02	kJ/mol	291.20	NIST Webbook
hfust	1.97	kJ/mol	297.10	NIST Webbook
hfust	2.06	kJ/mol	295.00	NIST Webbook
hfust	2.12	kJ/mol	261.30	NIST Webbook
hfust	2.06	kJ/mol	295.00	NIST Webbook
sfust	8.11	J/mol×K	261.30	NIST Webbook
sfust	6.98	J/mol×K	295.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	2.90	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C696719&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Heat capacities of selected cycloalcohols:	https://www.doi.org/10.1016/j.tca.2014.10.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol908.mol

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
hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume