

8-Oxabicyclo[5.1.0]octane

Other names:	Cycloheptane, 1,2-epoxy- Cycloheptene epoxide Cycloheptene oxide Epoxycycloheptane 1,2-Epoxycycloheptane cis-1,2-Epoxycycloheptane
Inchi:	InChI=1S/C7H12O/c1-2-4-6-7(8-6)5-3-1/h6-7H,1-5H2
InchiKey:	MLOZFLXCWGERSM-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	C1CCC2OC2CC1
Mol. weight [g/mol]:	112.17
CAS:	286-45-3

Physical Properties

Property code	Value	Unit	Source
chl	-4272.10 ± 3.10	kJ/mol	NIST Webbook
gf	19.24	kJ/mol	Joback Method
hf	-152.30 ± 3.10	kJ/mol	NIST Webbook
hfl	-197.50 ± 3.10	kJ/mol	NIST Webbook
hfus	13.93	kJ/mol	Joback Method
hvap	45.20 ± 0.40	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
log10ws	-1.85		Crippen Method
logp	1.718		Crippen Method
mcvol	93.640	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	408.53	K	Joback Method
tc	620.71	K	Joback Method
tf	224.06	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	189.08	J/mol×K	408.53	Joback Method
cpg	205.70	J/mol×K	443.89	Joback Method
cpg	221.26	J/mol×K	479.26	Joback Method
cpg	235.82	J/mol×K	514.62	Joback Method
cpg	249.44	J/mol×K	549.98	Joback Method
cpg	262.16	J/mol×K	585.35	Joback Method
cpg	274.04	J/mol×K	620.71	Joback Method
dvisc	0.0018676	Paxs	224.06	Joback Method
dvisc	0.0013582	Paxs	254.81	Joback Method
dvisc	0.0010578	Paxs	285.55	Joback Method
dvisc	0.0008649	Paxs	316.29	Joback Method
dvisc	0.0007328	Paxs	347.04	Joback Method
dvisc	0.0006379	Paxs	377.78	Joback Method
dvisc	0.0005670	Paxs	408.53	Joback Method

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=C286453&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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