8-Oxatricyclo[3,2,1,0(1,5)]octane

Inchi: InChI=1S/C7H12O/c1-2-6-4-5-7(3-1)8-6/h6-7H,1-5H2
InchiKey: AWEGTPPFDJUPRI-UHFFFAOYSA-N
Formula: C7H10O
SMILES: C1CC2CCC(C1)O2
Mol. weight [g/mol]: 110.15
CAS: 22341-17-9

Physical Properties

Property code	Value	Unit	Source
chl	-4174.30 ± 0.96	kJ/mol	NIST Webbook
gf	19.24	kJ/mol	Joback Method
hf	27.00	kJ/mol	NIST Webbook
hfl	-9.54	kJ/mol	NIST Webbook
hfus	13.93	kJ/mol	Joback Method
hvap	36.00 ± 1.30	kJ/mol	NIST Webbook
hvap	36.50	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
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	Pa×s	224.06	Joback Method
dvisc	0.0013582	Pa×s	254.81	Joback Method
dvisc	0.0010578	Pa×s	285.55	Joback Method
dvisc	0.0008649	Pa×s	316.29	Joback Method
dvisc	0.0007328	Pa×s	347.04	Joback Method
dvisc	0.0006379	Pa×s	377.78	Joback Method
dvisc	0.0005670	Pa×s	408.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22341179&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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