

cis-Oxolane-3,4-diol dinitrate

Inchi:	InChI=1S/C8H12O5/c1-5(9)12-7-3-11-4-8(7)13-6(2)10/h7-8H,3-4H2,1-2H3
InchiKey:	UTLGQZBGMVTJJZ-UHFFFAOYSA-N
Formula:	C8H12O5
SMILES:	CC(=O)OC1COCC1OC(C)=O
Mol. weight [g/mol]:	188.18
CAS:	85440-70-6

Physical Properties

Property code	Value	Unit	Source
chl	-3885.10 ± 3.70	kJ/mol	NIST Webbook
gf	-508.64	kJ/mol	Joback Method
hf	-789.91	kJ/mol	Joback Method
hfl	-978.00 ± 3.70	kJ/mol	NIST Webbook
hfus	25.04	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-0.10		Crippen Method
logp	-0.120		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	572.58	K	Joback Method
tc	781.77	K	Joback Method
tf	357.47	K	Joback Method
vc	0.492	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.96	J/mol×K	572.58	Joback Method
cpg	400.40	J/mol×K	746.90	Joback Method
cpg	389.54	J/mol×K	712.04	Joback Method
cpg	377.95	J/mol×K	677.17	Joback Method
cpg	365.65	J/mol×K	642.31	Joback Method
cpg	352.65	J/mol×K	607.44	Joback Method
cpg	410.53	J/mol×K	781.77	Joback Method

dvisc	0.0003459	Paxs	572.58	Joback Method
dvisc	0.0004213	Paxs	536.73	Joback Method
dvisc	0.0005278	Paxs	500.88	Joback Method
dvisc	0.0006846	Paxs	465.02	Joback Method
dvisc	0.0009275	Paxs	429.17	Joback Method
dvisc	0.0013282	Paxs	393.32	Joback Method
dvisc	0.0020438	Paxs	357.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85440706&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

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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