

trans-Oxolane-3,4-diol dinitrate

Inchi:	InChI=1S/C4H6N2O7/c7-5(8)12-3-1-11-2-4(3)13-6(9)10/h3-4H,1-2H2/t3-,4-/m0/s1
InchiKey:	NUPHETKTSSIAEZ-IMJSIDKUSA-N
Formula:	C4H6N2O7
SMILES:	O=[N+]([O-])OC1COCC1O[N+](=O)[O-]
Mol. weight [g/mol]:	194.10
CAS:	58690-46-3

Physical Properties

Property code	Value	Unit	Source
chl	-2045.50 ± 1.70	kJ/mol	NIST Webbook
gf	-213.38	kJ/mol	Joback Method
hf	-503.71	kJ/mol	Joback Method
hfl	-386.00 ± 1.70	kJ/mol	NIST Webbook
hfus	34.20	kJ/mol	Joback Method
hvap	66.96	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	-0.830		Crippen Method
mcvol	108.810	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
tb	677.00	K	Joback Method
tc	937.19	K	Joback Method
tf	499.75	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.80	J/mol×K	677.00	Joback Method
cpg	317.73	J/mol×K	720.36	Joback Method
cpg	327.71	J/mol×K	763.73	Joback Method
cpg	336.71	J/mol×K	807.09	Joback Method
cpg	344.73	J/mol×K	850.46	Joback Method
cpg	351.75	J/mol×K	893.82	Joback Method
cpg	357.76	J/mol×K	937.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58690463&Units=SI
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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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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