cis-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+
InchiKey: NUPHETKTSSIAEZ-ZXZARUISSA-N
Formula: C4H6N2O7
SMILES: O=[N+]([O-])OC1COCC1O[N+](=O)[O-]
Mol. weight [g/mol]: 194.10
CAS: 58690-45-2

Physical Properties

Property code	Value	Unit	Source
chs	-2025.50 ± 2.50	kJ/mol	NIST Webbook
gf	-213.38	kJ/mol	Joback Method
hf	-503.71	kJ/mol	Joback Method
hfs	-406.00 ± 2.50	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	m3/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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58690452&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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