1,2-Hexanediol, dinitrate

Other names: 1-nitrooxyhexan-2-yl nitrate
Inchi: InChI=1S/C6H12N2O6/c1-2-3-4-6(14-8(11)12)5-13-7(9)10/h6H,2-5H2,1H3
InchiKey: YUWYAYLMKPCSHB-UHFFFAOYSA-N
Formula: C6H12N2O6
SMILES: CCCCC(CO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 208.17

Physical Properties

Property code	Value	Unit	Source
gf	-141.70	kJ/mol	Joback Method
hf	-458.41	kJ/mol	Joback Method
hfus	32.87	kJ/mol	Joback Method
hvap	66.56	kJ/mol	Joback Method
log10ws	-3.10		Aqueous Solubility Prediction Method
logp	0.962		Crippen Method
mcvol	141.980	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1261.00		NIST Webbook
tb	684.76	K	Joback Method
tc	911.10	K	Joback Method
tf	474.06	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.10	J/mol×K	684.76	Joback Method
cpg	399.35	J/mol×K	722.48	Joback Method
cpg	409.85	J/mol×K	760.21	Joback Method
cpg	419.60	J/mol×K	797.93	Joback Method
cpg	428.59	J/mol×K	835.65	Joback Method
cpg	436.82	J/mol×K	873.37	Joback Method
cpg	444.29	J/mol×K	911.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume