1,8-Octanediol, dinitrate

Other names: 8-nitrooxyoctyl nitrate
Inchi: InChI=1S/C8H16N2O6/c11-9(12)15-7-5-3-1-2-4-6-8-16-10(13)14/h1-8H2
InchiKey: DCPXXVXZJCAQDR-UHFFFAOYSA-N
Formula: C8H16N2O6
SMILES: O=[N+]([O-])OCCCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]: 236.22

Physical Properties

Property code	Value	Unit	Source
gf	-122.42	kJ/mol	Joback Method
hf	-494.41	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-4.14		Aqueous Solubility Prediction Method
logp	1.744		Crippen Method
mcvol	170.160	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1647.00		NIST Webbook
tb	730.96	K	Joback Method
tc	946.13	K	Joback Method
tf	511.60	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.26	J/mol×K	730.96	Joback Method
cpg	501.49	J/mol×K	766.82	Joback Method
cpg	512.92	J/mol×K	802.68	Joback Method
cpg	523.54	J/mol×K	838.54	Joback Method
cpg	533.37	J/mol×K	874.41	Joback Method
cpg	542.39	J/mol×K	910.27	Joback Method
cpg	550.63	J/mol×K	946.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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