1,7-Heptanediol, dinitrate

Other names: 7-nitrooxyheptyl nitrate
Inchi: InChI=1S/C7H14N2O6/c10-8(11)14-6-4-2-1-3-5-7-15-9(12)13/h1-7H2
InchiKey: WNRZBFNPJUBEMS-UHFFFAOYSA-N
Formula: C7H14N2O6
SMILES: O=[N+]([O-])OCCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]: 222.20

Physical Properties

Property code	Value	Unit	Source
gf	-130.84	kJ/mol	Joback Method
hf	-473.77	kJ/mol	Joback Method
hfus	38.98	kJ/mol	Joback Method
hvap	69.18	kJ/mol	Joback Method
log10ws	-3.40		Aqueous Solubility Prediction Method
logp	1.353		Crippen Method
mcvol	156.070	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1543.00		NIST Webbook
tb	708.08	K	Joback Method
tc	926.47	K	Joback Method
tf	500.33	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.72	J/mol×K	708.08	Joback Method
cpg	449.39	J/mol×K	744.48	Joback Method
cpg	460.30	J/mol×K	780.88	Joback Method
cpg	470.45	J/mol×K	817.28	Joback Method
cpg	479.84	J/mol×K	853.68	Joback Method
cpg	488.47	J/mol×K	890.08	Joback Method
cpg	496.34	J/mol×K	926.47	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=R496665&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

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