

1,6-Hexanediol, dinitrate

Other names:	6-nitrooxyhexyl nitrate
Inchi:	InChI=1S/C6H12N2O6/c9-7(10)13-5-3-1-2-4-6-14-8(11)12/h1-6H2
InchiKey:	BQJMULTPFAUGVGY-UHFFFAOYSA-N
Formula:	C6H12N2O6
SMILES:	O=[N+](O-)[O-]OCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	208.17

Physical Properties

Property code	Value	Unit	Source
gf	-139.26	kJ/mol	Joback Method
hf	-453.13	kJ/mol	Joback Method
hfus	36.39	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-2.77		Aqueous Solubility Prediction Method
logp	0.963		Crippen Method
mcvol	141.980	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	1438.00		NIST Webbook
tb	685.20	K	Joback Method
tc	907.25	K	Joback Method
tf	489.06	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.53	J/mol×K	685.20	Joback Method
cpg	398.53	J/mol×K	722.21	Joback Method
cpg	408.83	J/mol×K	759.22	Joback Method
cpg	418.42	J/mol×K	796.22	Joback Method
cpg	427.29	J/mol×K	833.23	Joback Method
cpg	435.45	J/mol×K	870.24	Joback Method
cpg	442.88	J/mol×K	907.25	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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