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: BQJMULPFAUGVGY-UHFFFAOYSA-N
Formula: C6H12N2O6
SMILES: O=[N+]([O-])OCCCCCCO[N+](=O)[O-]
Mol. weight [g/mol]: 208.17
CAS: 3457-93-0

Physical Properties

Property code	Value	Unit	Source
hf	-302.55	kJ/mol	Cheméo Relay (1.0)
hfus	36.39	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Cheméo Relay (1.0)
ie	10.89	eV	Cheméo Relay (1.0)
log10ws	-2.77		Aqueous Solubility Prediction Method
logp	0.963		Crippen Method
mcvol	141.980	ml/mol	McGowan Method
tb	502.10	K	Cheméo Relay (1.0)
tf	276.00	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3457930&Units=SI&Mask=3FFF
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point