isosorbide dinitrate

Inchi: InChI=1S/C6H8N2O8/c9-7(10)15-3-1-13-6-4(16-8(11)12)2-14-5(3)6/h3-6H,1-2H2
InchiKey: MOYKHGMNXAOIAT-UHFFFAOYSA-N
Formula: C6H8N2O8
SMILES: O=[N+]([O-])OC1COC2C(O[N+](=O)[O-])COC12
Mol. weight [g/mol]: 236.14

Physical Properties

Property code	Value	Unit	Source
gf	-229.62	kJ/mol	Joback Method
hf	-624.53	kJ/mol	Joback Method
hfus	46.56	kJ/mol	Joback Method
hvap	75.52	kJ/mol	Joback Method
log10ws	-2.63		Aqueous Solubility Prediction Method
logp	-1.062		Crippen Method
mcvol	132.000	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
tb	751.78	K	Joback Method
tc	1012.88	K	Joback Method
tf	562.56	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.21	J/mol×K	751.78	Joback Method
cpg	432.32	J/mol×K	795.30	Joback Method
cpg	443.23	J/mol×K	838.81	Joback Method
cpg	452.98	J/mol×K	882.33	Joback Method
cpg	461.59	J/mol×K	925.84	Joback Method
cpg	469.10	J/mol×K	969.36	Joback Method
cpg	475.52	J/mol×K	1012.88	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume