1,3-Butanediol dinitrate

Other names: 4-nitrooxybutan-2-yl nitrate
Inchi: InChI=1S/C4H8N2O6/c1-4(12-6(9)10)2-3-11-5(7)8/h4H,2-3H2,1H3
InchiKey: DGFBULNMARLFTH-UHFFFAOYSA-N
Formula: C4H8N2O6
SMILES: CC(CCO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 180.12
CAS: 6423-44-5

Physical Properties

Property code	Value	Unit	Source
chl	-2377.00	kJ/mol	NIST Webbook
gf	-158.54	kJ/mol	Joback Method
hf	-417.13	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	62.11	kJ/mol	Joback Method
log10ws	-1.66		Aqueous Solubility Prediction Method
logp	0.182		Crippen Method
mcvol	113.800	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1123.00		NIST Webbook
tb	639.00	K	Joback Method
tc	874.34	K	Joback Method
tf	253.40 ± 0.10	K	NIST Webbook
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.08	J/mol×K	639.00	Joback Method
cpg	301.65	J/mol×K	678.22	Joback Method
cpg	310.61	J/mol×K	717.45	Joback Method

cpg	318.93	J/mol×K	756.67	Joback Method
cpg	326.61	J/mol×K	795.89	Joback Method
cpg	333.63	J/mol×K	835.11	Joback Method
cpg	339.98	J/mol×K	874.34	Joback Method
hvapt	71.40 ± 7.10	kJ/mol	303.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6423445&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

chl: Standard liquid enthalpy of combustion
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
hvapt: Enthalpy of vaporization at a given temperature
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