2,3-Butanediol, dinitrate

Other names: 2,3-Butylene glycol dinitrate
3-nitrooxybutan-2-yl nitrate
Inchi: InChI=1S/C4H8N2O6/c1-3(11-5(7)8)4(2)12-6(9)10/h3-4H,1-2H3
InchiKey: RVDDYBGRQLZMSB-UHFFFAOYSA-N
Formula: C4H8N2O6
SMILES: CC(O[N+](=O)[O-])C(C)O[N+](=O)[O-]
Mol. weight [g/mol]: 180.12
CAS: 6423-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-160.98	kJ/mol	Joback Method
hf	-422.41	kJ/mol	Joback Method
hfus	24.17	kJ/mol	Joback Method
hvap	61.72	kJ/mol	Joback Method
log10ws	-1.89		Aqueous Solubility Prediction Method
logp	0.180		Crippen Method
mcvol	113.800	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	638.56	K	Joback Method
tc	878.95	K	Joback Method
tf	436.52	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.63	J/mol×K	638.56	Joback Method
cpg	302.45	J/mol×K	678.62	Joback Method
cpg	311.61	J/mol×K	718.69	Joback Method
cpg	320.10	J/mol×K	758.75	Joback Method
cpg	327.90	J/mol×K	798.82	Joback Method
cpg	335.00	J/mol×K	838.88	Joback Method

cpg	341.39	J/mol×K	878.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6423456&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

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