1,4-Butanediol, dinitrate

Other names:	1,4-Butylene glycol dinitrate
	4-nitrooxybutyl nitrate
	Tetramethylene dinitrate
	Tetramethylene nitrate
Inchi:	InChI=1S/C4H8N2O6/c7-5(8)11-3-1-2-4-12-6(9)10/h1-4H2
InchiKey:	QELUAJBXJAWSRC-UHFFFAOYSA-N
Formula:	C4H8N2O6
SMILES:	O=[N+]([O-])OCCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	180.12
CAS:	3457-91-8

Physical Properties

Property code	Value	Unit	Source
chl	-2387.00	kJ/mol	NIST Webbook
gf	-156.10	kJ/mol	Joback Method
hf	-411.85	kJ/mol	Joback Method
hfl	-331.00	kJ/mol	NIST Webbook
hfl	-274.00	kJ/mol	NIST Webbook
hfus	31.21	kJ/mol	Joback Method
hvap	62.50	kJ/mol	Joback Method
log10ws	-1.68		Aqueous Solubility Prediction Method
logp	0.183		Crippen Method
mcvol	113.800	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1213.00		NIST Webbook
tb	639.44	K	Joback Method
tc	869.91	K	Joback Method
tf	285.00 ± 0.10	K	NIST Webbook
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	291.53	J/mol×K	639.44	Joback Method
cpg	300.86	J/mol×K	677.85	Joback Method
cpg	309.61	J/mol×K	716.26	Joback Method
cpg	317.77	J/mol×K	754.67	Joback Method
cpg	325.33	J/mol×K	793.08	Joback Method
cpg	332.27	J/mol×K	831.50	Joback Method
cpg	338.58	J/mol×K	869.91	Joback Method
hvapt	57.40 ± 0.80	kJ/mol	303.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3457918&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

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
hfl: Liquid phase 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