1,2,4-Butanetriol, trinitrate

Other names: Butane-1,2,4-triyl nitrate
butane-1,2,4-triyl trinitrate
Inchi: InChI=1S/C4H7N3O9/c8-5(9)14-2-1-4(16-7(12)13)3-15-6(10)11/h4H,1-3H2
InchiKey: RDLIBIDNLZPAQD-UHFFFAOYSA-N
Formula: C4H7N3O9
SMILES: O=[N+]([O-])OCCC(CO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 241.11
CAS: 6659-60-5

Physical Properties

Property code	Value	Unit	Source
chl	-2311.00	kJ/mol	NIST Webbook
chl	-2177.00	kJ/mol	NIST Webbook
chs	-2175.70	kJ/mol	NIST Webbook
gf	-227.99	kJ/mol	Joback Method
hf	-560.11	kJ/mol	Joback Method
hfl	-414.00	kJ/mol	NIST Webbook
hfus	40.24	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	-0.630		Crippen Method
mcvol	137.090	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
tb	813.26	K	Joback Method
tc	1063.27	K	Joback Method
tf	617.36	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.92	J/mol×K	813.26	Joback Method

cpg	400.77	J/mol×K	854.93	Joback Method
cpg	407.66	J/mol×K	896.60	Joback Method
cpg	413.56	J/mol×K	938.26	Joback Method
cpg	418.44	J/mol×K	979.93	Joback Method
cpg	422.28	J/mol×K	1021.60	Joback Method
cpg	425.03	J/mol×K	1063.27	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6659605&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid 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
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

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