butane-1,2,3-triyl trinitrate

Other names: 1,2,3-Butanetriol, trinitrate
Inchi: InChI=1S/C4H7N3O9/c1-3(15-6(10)11)4(16-7(12)13)2-14-5(8)9/h3-4H,2H2,1H3
InchiKey: GIFRMMSPDQZIHL-UHFFFAOYSA-N
Formula: C4H7N3O9
SMILES: CC(O[N+](=O)[O-])C(CO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 241.11
CAS: 84002-64-2

Physical Properties

Property code	Value	Unit	Source
chl	-2175.70	kJ/mol	NIST Webbook
gf	-230.43	kJ/mol	Joback Method
hf	-565.39	kJ/mol	Joback Method
hfus	36.72	kJ/mol	Joback Method
hvap	80.72	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	-0.632		Crippen Method
mcvol	137.090	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	812.82	K	Joback Method
tc	1067.41	K	Joback Method
tf	602.36	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.57	J/mol×K	812.82	Joback Method
cpg	401.55	J/mol×K	855.25	Joback Method
cpg	408.52	J/mol×K	897.68	Joback Method
cpg	414.44	J/mol×K	940.12	Joback Method
cpg	419.29	J/mol×K	982.55	Joback Method
cpg	423.03	J/mol×K	1024.98	Joback Method
cpg	425.63	J/mol×K	1067.41	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C84002642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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