

Butanoic acid, 4,4,4-trinitro-, 2,2,2-trinitroethyl ester

Other names:	Butyric acid, 4,4,4-trinitro-, 2,2,2-trinitroethyl ester 4,4,4-Trinitrobutyric acid 2,2,2-trinitroethyl ester
Inchi:	InChI=1S/C6H6N6O14/c13-4(1-2-5(7(14)15,8(16)17)9(18)19)26-3-6(10(20)21,11(22)23)
InchiKey:	IAVWMTSJZOZYCU-UHFFFAOYSA-N
Formula:	C6H6N6O14
SMILES:	O=C(CCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-])OCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	386.14
CAS:	866-65-9

Physical Properties

Property code	Value	Unit	Source
gf	-15.30	kJ/mol	Joback Method
hf	-494.03	kJ/mol	Joback Method
hfus	67.42	kJ/mol	Joback Method
hvap	135.06	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	-1.722		Crippen Method
mcvol	207.360	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	1317.55	K	Joback Method
tc	1631.23	K	Joback Method
tf	1096.04	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.20	J/mol×K	1317.55	Joback Method
cpg	650.44	J/mol×K	1369.83	Joback Method
cpg	655.09	J/mol×K	1422.11	Joback Method
cpg	660.40	J/mol×K	1474.39	Joback Method
cpg	666.57	J/mol×K	1526.67	Joback Method
cpg	673.82	J/mol×K	1578.95	Joback Method
cpg	682.39	J/mol×K	1631.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C866659&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

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