Butyronitrile, 4,4,4-trinitro-

Inchi: InChI=1S/C4H4N4O6/c5-3-1-2-4(6(9)10,7(11)12)8(13)14/h1-2H2
InchiKey: XOUYZYXSMDSAOU-UHFFFAOYSA-N
Formula: C4H4N4O6
SMILES: N#CCCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 204.10
CAS: 15473-29-7

Physical Properties

Property code	Value	Unit	Source
gf	225.47	kJ/mol	Joback Method
hf	-2.04	kJ/mol	Joback Method
hfs	3.40 ± 1.40	kJ/mol	NIST Webbook
hfus	34.29	kJ/mol	Joback Method
hvap	83.45	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	-0.226		Crippen Method
mcvol	120.860	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	845.29	K	Joback Method
tc	1126.15	K	Joback Method
tf	633.08	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.21	J/mol×K	845.29	Joback Method
cpg	331.74	J/mol×K	892.10	Joback Method
cpg	336.66	J/mol×K	938.91	Joback Method
cpg	341.07	J/mol×K	985.72	Joback Method
cpg	345.08	J/mol×K	1032.53	Joback Method
cpg	348.78	J/mol×K	1079.34	Joback Method
cpg	352.28	J/mol×K	1126.15	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=C15473297&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume