

Butyramide, 4,4,4-trinitro-

Inchi:	InChI=1S/C4H6N4O7/c5-3(9)1-2-4(6(10)11,7(12)13)8(14)15/h1-2H2,(H2,5,9)
InchiKey:	HNLKKBHYPDVWGZ-UHFFFAOYSA-N
Formula:	C4H6N4O7
SMILES:	NC(=O)CCC([N+](=O)[O-])([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	222.11
CAS:	13000-42-5

Physical Properties

Property code	Value	Unit	Source
gf	29.82	kJ/mol	Joback Method
hf	-245.71	kJ/mol	Joback Method
hfs	-214.60 ± 1.20	kJ/mol	NIST Webbook
hfus	39.58	kJ/mol	Joback Method
hvap	90.36	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	-1.264		Crippen Method
mcvol	131.030	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
tb	869.61	K	Joback Method
tc	1148.79	K	Joback Method
tf	701.28	K	Joback Method
vc	0.529	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.50	J/mol×K	869.61	Joback Method
cpg	381.57	J/mol×K	916.14	Joback Method
cpg	386.95	J/mol×K	962.67	Joback Method
cpg	391.75	J/mol×K	1009.20	Joback Method
cpg	396.06	J/mol×K	1055.73	Joback Method
cpg	399.99	J/mol×K	1102.26	Joback Method
cpg	403.64	J/mol×K	1148.79	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=C13000425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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