1-Butanamine, N-nitro-

Other names: n-Butylnitramine
Inchi: InChI=1S/C4H10N2O2/c1-2-3-4-5-6(7)8/h5H,2-4H2,1H3
InchiKey: FCLOSAGZCUDMFV-UHFFFAOYSA-N
Formula: C4H10N2O2
SMILES: CCCCN[N+](=O)[O-]
Mol. weight [g/mol]: 118.13
CAS: 3182-75-0

Physical Properties

Property code	Value	Unit	Source
chl	-2887.00	kJ/mol	NIST Webbook
gf	107.74	kJ/mol	Joback Method
hf	-83.18	kJ/mol	Joback Method
hfus	22.58	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	0.568		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	492.93	K	Joback Method
tc	701.96	K	Joback Method
tf	331.11	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.31	J/mol×K	492.93	Joback Method
cpg	219.21	J/mol×K	527.77	Joback Method
cpg	228.58	J/mol×K	562.61	Joback Method
cpg	237.45	J/mol×K	597.44	Joback Method
cpg	245.83	J/mol×K	632.28	Joback Method
cpg	253.74	J/mol×K	667.12	Joback Method
cpg	261.19	J/mol×K	701.96	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=C3182750&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