N-Butyl-N-(2-hydroxyethyl)nitramine, nitrate

Other names: N-Butyl-N-(2-hydroxyethyl)nitramine, dinitrate (ester)
N-Butyl-2-nitratoethylnitramine
2-(butylnitroamino)ethyl nitrate
Inchi: InChI=1S/C6H13N3O5/c1-2-3-4-7(8(10)11)5-6-14-9(12)13/h2-6H2,1H3
InchiKey: TUIUTESNLKHOHQ-UHFFFAOYSA-N
Formula: C6H13N3O5
SMILES: CCCCN(CCO[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 207.19

Physical Properties

Property code	Value	Unit	Source
chl	-4026.60	kJ/mol	NIST Webbook
hf	-172.68	kJ/mol	Cheméo Relay (1.0)
hfl	-192.47	kJ/mol	NIST Webbook
hfus	38.23	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-2.32		Cheméo Relay (1.0)
logp	0.489		Crippen Method
mcvol	146.090	ml/mol	McGowan Method
tb	518.55	K	Cheméo Relay (1.0)
tf	262.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.03	J/mol×K	675.22	Joback Method
cpg	412.58	J/mol×K	712.15	Joback Method
cpg	423.35	J/mol×K	749.09	Joback Method
cpg	433.37	J/mol×K	786.02	Joback Method
cpg	442.66	J/mol×K	822.96	Joback Method
cpg	451.24	J/mol×K	859.89	Joback Method
cpg	459.15	J/mol×K	896.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82486826&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point