Ethanol, 2-(butylnitroamino)-, 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]: 207.18
CAS: 82486-82-6

Physical Properties

Property code	Value	Unit	Source
gf	76.52	kJ/mol	Joback Method
hf	-253.38	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	66.58	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	0.489		Crippen Method
mcvol	146.090	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	675.22	K	Joback Method
tc	896.83	K	Joback Method
tf	499.30	K	Joback Method
vc	0.572	m3/kmol	Joback Method

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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