Di-n-butylnitramine

Other names:	Dibutylamine, N-nitro- Dibutylnitramine N-Nitrodibutylamine Di-n-butylnitramine
Inchi:	InChI=1S/C8H18N2O2/c1-3-5-7-9(10(11)12)8-6-4-2/h3-8H2,1-2H3
InchiKey:	IBFAEPSQNZNTBK-UHFFFAOYSA-N
Formula:	C8H18N2O2
SMILES:	CCCCN(CCCC)[N+](=O)[O-]
Mol. weight [g/mol]:	174.24

Physical Properties

Property code	Value	Unit	Source
af	0.6227		Cheméo Relay (1.0)
chl	-5510.70	kJ/mol	NIST Webbook
hfus	30.86	kJ/mol	Joback Method
hvap	56.09	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	Cheméo Relay (1.0)
log10ws	-2.86		Cheméo Relay (1.0)
logp	2.080		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	521.57	K	Cheméo Relay (1.0)
tc	695.66	K	Cheméo Relay (1.0)
tf	262.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.10	J/mol×K	546.72	Joback Method
cpg	387.42	J/mol×K	579.03	Joback Method
cpg	400.99	J/mol×K	611.34	Joback Method
cpg	413.85	J/mol×K	643.65	Joback Method
cpg	426.02	J/mol×K	675.96	Joback Method
cpg	437.52	J/mol×K	708.27	Joback Method

cpg	448.40	J/mol×K	740.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4164312&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

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point