N-Nitrosodibutylamine, HFBA-derivative

Inchi: InChI=1S/C16H14F14N2O2/c1-3-5-7-31(8-6-4-2)32(9(33)11(17,18)13(21,22)15(25,26)27
InchiKey: ZZJBFLNEZLNXNT-CGXWXWIYSA-N
Formula: C16H14F14N2O2
SMILES: CCC=CN(C=CCC)N(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 532.27

Physical Properties

Property code	Value	Unit	Source
gf	-2502.30	kJ/mol	Joback Method
hf	-3027.27	kJ/mol	Joback Method
hfus	45.48	kJ/mol	Joback Method
hvap	49.49	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.072		Crippen Method
mcvol	275.580	ml/mol	McGowan Method
pc	1079.22	kPa	Joback Method
rinpol	1290.00		NIST Webbook
tb	676.82	K	Joback Method
tc	832.22	K	Joback Method
tf	447.50	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.29	J/mol×K	676.82	Joback Method
cpg	847.68	J/mol×K	702.72	Joback Method
cpg	859.15	J/mol×K	728.62	Joback Method
cpg	869.78	J/mol×K	754.52	Joback Method
cpg	879.65	J/mol×K	780.42	Joback Method
cpg	888.87	J/mol×K	806.32	Joback Method
cpg	897.51	J/mol×K	832.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579903&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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