N-Nitrosodipropylamine, HFBA-derivative

Inchi: InChI=1S/C14H10F14N2O2/c1-3-5-29(6-4-2)30(7(31)9(15,16)11(19,20)13(23,24)25)8(32
InchiKey: SNQZPUKWJOYAKK-CIIODKQPSA-N
Formula: C14H10F14N2O2
SMILES: CC=CN(C=CC)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]: 504.22

Physical Properties

Property code	Value	Unit	Source
gf	-2519.14	kJ/mol	Joback Method
hf	-2985.99	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	45.04	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.292		Crippen Method
mcvol	247.400	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	1190.00		NIST Webbook
tb	631.06	K	Joback Method
tc	781.65	K	Joback Method
tf	424.96	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.12	J/mol×K	631.06	Joback Method
cpg	741.94	J/mol×K	656.16	Joback Method
cpg	752.83	J/mol×K	681.26	Joback Method
cpg	762.85	J/mol×K	706.36	Joback Method
cpg	772.09	J/mol×K	731.46	Joback Method
cpg	780.62	J/mol×K	756.56	Joback Method
cpg	788.52	J/mol×K	781.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579938&Units=SI

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