

N,N-Diethyl 1,1,2,3,3,3-hexafluoropropylamine

Inchi:	InChI=1S/C7H11F6N/c1-3-14(4-2)7(12,13)5(8)6(9,10)11/h5H,3-4H2,1-2H3
InchiKey:	BNTFCVMJHBNJAR-UHFFFAOYSA-N
Formula:	C7H11F6N
SMILES:	CCN(CC)C(F)(F)C(F)C(F)(F)F
Mol. weight [g/mol]:	223.16
CAS:	309-88-6

Physical Properties

Property code	Value	Unit	Source
gf	-1046.78	kJ/mol	Joback Method
hf	-1319.72	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	25.34	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.821		Crippen Method
mcvol	130.090	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
tb	360.72	K	Joback Method
tc	497.63	K	Joback Method
tf	194.50	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.54	J/molxK	360.72	Joback Method
cpg	283.30	J/molxK	383.54	Joback Method
cpg	295.45	J/molxK	406.36	Joback Method
cpg	307.02	J/molxK	429.17	Joback Method
cpg	318.01	J/molxK	451.99	Joback Method
cpg	328.45	J/molxK	474.81	Joback Method
cpg	338.37	J/molxK	497.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	329.50 ± 0.50	K	7.70	NIST Webbook

Sources

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=C309886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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