

Trifluoroacetamide, N-cyclohexyl-N-phenyl-

Other names:	N-Phenylcyclohexylamine, TFA
Inchi:	InChI=1S/C14H16F3NO/c15-14(16,17)13(19)18(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1,3-
InchiKey:	SVDOUZCIIWSZAX-UHFFFAOYSA-N
Formula:	C14H16F3NO
SMILES:	O=C(N(c1ccccc1)C1CCCCC1)C(F)(F)F
Mol. weight [g/mol]:	271.28

Physical Properties

Property code	Value	Unit	Source
gf	-395.87	kJ/mol	Joback Method
hf	-683.57	kJ/mol	Joback Method
hfus	24.34	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.915		Crippen Method
mvol	190.360	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
tb	626.84	K	Joback Method
tc	842.69	K	Joback Method
tf	367.93	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.47	J/molxK	626.84	Joback Method
cpg	542.02	J/molxK	662.82	Joback Method
cpg	559.13	J/molxK	698.79	Joback Method
cpg	574.90	J/molxK	734.77	Joback Method
cpg	589.41	J/molxK	770.74	Joback Method
cpg	602.74	J/molxK	806.72	Joback Method
cpg	614.98	J/molxK	842.69	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=U328355&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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