Trifluoroacetamide, N-(1-cyclohexylethyl)

Inchi: InChI=1S/C10H16F3NO/c1-7(8-5-3-2-4-6-8)14-9(15)10(11,12)13/h7-8H,2-6H2,1H3,(H,14
InchiKey: OGMDDSGBDBOSPC-UHFFFAOYSA-N
Formula: C10H16F3NO
SMILES: CC(NC(=O)C(F)(F)F)C1CCCCC1
Mol. weight [g/mol]: 223.24

Physical Properties

Property code	Value	Unit	Source
gf	-565.79	kJ/mol	Joback Method
hf	-856.88	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.634		Crippen Method
mcvol	157.760	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1227.00		NIST Webbook
rinpol	1227.00		NIST Webbook
tb	545.93	K	Joback Method
tc	740.63	K	Joback Method
tf	301.62	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.15	J/mol×K	545.93	Joback Method
cpg	427.22	J/mol×K	578.38	Joback Method
cpg	443.24	J/mol×K	610.83	Joback Method
cpg	458.26	J/mol×K	643.28	Joback Method
cpg	472.32	J/mol×K	675.73	Joback Method
cpg	485.47	J/mol×K	708.18	Joback Method
cpg	497.74	J/mol×K	740.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R74074&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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