Acetamide, N-(3-chlorophenyl)-2,2,2-trifluoro-

Other names: N-(3-Chlorophenyl)-2,2,2-trifluoroacetamide
Inchi: InChI=1S/C8H5ClF3NO/c9-5-2-1-3-6(4-5)13-7(14)8(10,11)12/h1-4H,(H,13,14)
InchiKey: VRKVCIVKSRGSLU-UHFFFAOYSA-N
Formula: C8H5ClF3NO
SMILES: O=C(Nc1cccc(Cl)c1)C(F)(F)F
Mol. weight [g/mol]: 223.58

Physical Properties

Property code	Value	Unit	Source
gf	-513.79	kJ/mol	Joback Method
hf	-655.32	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	50.16	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.841		Crippen Method
mcvol	128.920	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1314.00		NIST Webbook
tb	550.15	K	Joback Method
tc	758.89	K	Joback Method
tf	355.56	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.67	J/mol×K	550.15	Joback Method
cpg	296.59	J/mol×K	584.94	Joback Method
cpg	305.72	J/mol×K	619.73	Joback Method
cpg	314.11	J/mol×K	654.52	Joback Method
cpg	321.81	J/mol×K	689.31	Joback Method
cpg	328.86	J/mol×K	724.10	Joback Method
cpg	335.31	J/mol×K	758.89	Joback Method

Sources

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=U373268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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