2,2,2-Trichloro-3'-(trifluoromethyl)acetanilide

Other names: 3'-Trifluoromethyl-2,2,2-trichloroacetanilide
Inchi: InChI=1S/C9H5Cl3F3NO/c10-8(11,12)7(17)16-6-3-1-2-5(4-6)9(13,14)15/h1-4H,(H,16,17)
InchiKey: KQIOOEOHDXWXQY-UHFFFAOYSA-N
Formula: C9H5Cl3F3NO
SMILES: O=C(Nc1cccc(C(F)(F)F)c1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 306.50
CAS: 1939-29-3

Physical Properties

Property code	Value	Unit	Source
gf	-526.39	kJ/mol	Joback Method
hf	-716.19	kJ/mol	Joback Method
hfus	26.42	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.014		Crippen Method
mcvol	167.490	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	644.66	K	Joback Method
tc	870.03	K	Joback Method
tf	429.09	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.62	J/mol×K	644.66	Joback Method
cpg	388.66	J/mol×K	682.22	Joback Method
cpg	396.77	J/mol×K	719.78	Joback Method
cpg	404.03	J/mol×K	757.35	Joback Method
cpg	410.55	J/mol×K	794.91	Joback Method
cpg	416.42	J/mol×K	832.47	Joback Method
cpg	421.72	J/mol×K	870.03	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=C1939293&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume