

2,2,2-Trichloro-3'-trifluoromethylacetanilide

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

Physical Properties

Property code	Value	Unit	Source
hf	-789.72	kJ/mol	Cheméo Relay (1.0)
hfus	26.42	kJ/mol	Joback Method
hvap	68.88	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-4.59		Cheméo Relay (1.0)
logp	4.014		Crippen Method
mcvol	167.490	ml/mol	McGowan Method
tb	545.42	K	Cheméo Relay (1.0)
tf	357.65	K	Cheméo Relay (1.0)

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:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1939293&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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