

Ethyl 4-chloro-3-trifluoromethylcarbanilate

Inchi:	InChI=1S/C10H9ClF3NO2/c1-2-17-9(16)15-6-3-4-8(11)7(5-6)10(12,13)14/h3-5H,2H2,1H
InchiKey:	BAFPGGUKCVCSKG-UHFFFAOYSA-N
Formula:	C10H9ClF3NO2
SMILES:	CCOC(=O)Nc1ccc(Cl)c(C(F)(F)F)c1
Mol. weight [g/mol]:	267.63
CAS:	18585-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-611.58	kJ/mol	Joback Method
hf	-840.29	kJ/mol	Joback Method
hfus	28.83	kJ/mol	Joback Method
hvap	57.68	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.927		Crippen Method
mcvol	162.970	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	623.31	K	Joback Method
tc	824.81	K	Joback Method
tf	412.85	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.92	J/molxK	623.31	Joback Method
cpg	410.89	J/molxK	656.89	Joback Method
cpg	421.12	J/molxK	690.48	Joback Method
cpg	430.65	J/molxK	724.06	Joback Method
cpg	439.51	J/molxK	757.65	Joback Method
cpg	447.71	J/molxK	791.23	Joback Method
cpg	455.30	J/molxK	824.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18585063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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