chlorfenethol, TFA

Inchi: InChI=1S/C16H11Cl2F3O2/c1-15(23-14(22)16(19,20)21,10-2-6-12(17)7-3-10)11-4-8-13(

InchiKey: DGCXBBRJRFHPCX-UHFFFAOYSA-N

Formula: C16H11Cl2F3O2

SMILES: CC(OC(=O)C(F)(F)F)(c1ccc(Cl)cc1)c1ccc(Cl)cc1

Mol. weight [g/mol]: 363.16

Physical Properties

Property code	Value	Unit	Source
gf	-547.13	kJ/mol	Joback Method
hf	-805.56	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.362		Crippen Method
mcvol	226.010	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1898.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	771.30	K	Joback Method
tc	1005.56	K	Joback Method
tf	486.57	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.08	J/mol×K	771.30	Joback Method
cpg	605.95	J/mol×K	810.34	Joback Method
cpg	616.71	J/mol×K	849.39	Joback Method
cpg	626.49	J/mol×K	888.43	Joback Method
cpg	635.37	J/mol×K	927.48	Joback Method
cpg	643.46	J/mol×K	966.52	Joback Method
cpg	650.88	J/mol×K	1005.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522120&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