

chlorbenzilate, TFA

Inchi:

InChI=1S/C18H13Cl2F3O4/c1-2-26-15(24)17(27-16(25)18(21,22)23,11-3-7-13(19)8-4-11

InchiKey:

SXNWERJLQQIYBL-UHFFFAOYSA-N

Formula:

C18H13Cl2F3O4

SMILES:

CCOC(=O)C(OC(=O)C(F)(F)F)(c1ccc(Cl)cc1)c1ccc(Cl)cc1

Mol. weight [g/mol]:

421.19

Physical Properties

Property code	Value	Unit	Source
gf	-764.21	kJ/mol	Joback Method
hf	-1091.64	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	83.58	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.906		Crippen Method
mcvol	261.630	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2011.00		NIST Webbook
tb	893.35	K	Joback Method
tc	1124.44	K	Joback Method
tf	581.27	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.09	J/molxK	893.35	Joback Method
cpg	745.17	J/molxK	931.86	Joback Method
cpg	754.23	J/molxK	970.38	Joback Method
cpg	762.36	J/molxK	1008.89	Joback Method
cpg	769.64	J/molxK	1047.41	Joback Method
cpg	776.15	J/molxK	1085.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522115&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

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