2(2,2,2-trifluoroethyl)-amino--5-chloro-benzophen (TCB)

Other Names: 2-(2,2,2-Trifluoroethylamino)-5-chlorobenzophenone
Inchi: InChI=1S/C15H11ClF3NO/c16-11-6-7-13(20-9-15(17,18)19)12(8-11)14(21)10-4-2-1-3-5-
InchiKey: MKBQTVZIYPYTSC-UHFFFAOYSA-N
Formula: C15H11ClF3NO
SMILES: O=C(c1ccccc1)c1cc(Cl)ccc1NCC(F)(F)F
Mol. weight [g/mol]: 313.70

Physical Properties

Property code	Value	Unit	Source
gf	-352.07	kJ/mol	Joback Method
hf	-574.74	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	68.68	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.545		Crippen Method
mcvol	203.790	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2000.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	741.97	K	Joback Method
tc	967.16	K	Joback Method
tf	473.39	K	Joback Method
vc	0.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.36	J/mol×K	741.97	Joback Method
cpg	553.52	J/mol×K	779.50	Joback Method
cpg	564.65	J/mol×K	817.03	Joback Method
cpg	574.83	J/mol×K	854.56	Joback Method

cpg	584.15	J/mol×K	892.09	Joback Method
cpg	592.69	J/mol×K	929.63	Joback Method
cpg	600.55	J/mol×K	967.16	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=R42522&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume