2-(2,2,2-trifluoroethyl)-5-chloro-2'-fluorobenzophe (CFTB)

Inchi: InChI=1S/C15H9ClF4O/c16-10-6-5-9(8-15(18,19)20)12(7-10)14(21)11-3-1-2-4-13(11)17/

InchiKey: SUCZMAOZMIDABG-UHFFFAOYSA-N

Formula: C15H9ClF4O

SMILES: O=C(c1ccccc1F)c1cc(Cl)ccc1CC(F)(F)F

Mol. weight [g/mol]: 316.68

Physical Properties

Property code	Value	Unit	Source
gf	-645.90	kJ/mol	Joback Method
hf	-835.79	kJ/mol	Joback Method
hfus	32.22	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.815		Crippen Method
mcvol	195.580	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2395.00		NIST Webbook
tb	696.05	K	Joback Method
tc	914.01	K	Joback Method
tf	433.84	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.35	J/mol×K	696.05	Joback Method
cpg	510.46	J/mol×K	732.38	Joback Method
cpg	521.59	J/mol×K	768.70	Joback Method
cpg	531.82	J/mol×K	805.03	Joback Method
cpg	541.21	J/mol×K	841.36	Joback Method
cpg	549.82	J/mol×K	877.68	Joback Method
cpg	557.73	J/mol×K	914.01	Joback Method

Sources

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=R522239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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