2-Hydroxy-4'-trifluoromethyl-4-methoxybenzophe

Inchi: InChI=1S/C15H11F3O3/c1-21-11-6-7-12(13(19)8-11)14(20)9-2-4-10(5-3-9)15(16,17)18/h
InchiKey: SSMMHXAIFJLDSQ-UHFFFAOYSA-N
Formula: C15H11F3O3
SMILES: COc1ccc(C(=O)c2ccc(C(F)(F)F)cc2)c(O)c1
Mol. weight [g/mol]: 296.24
CAS: 7396-90-9

Physical Properties

Property code	Value	Unit	Source
gf	-689.15	kJ/mol	Joback Method
hf	-922.00	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	73.28	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.651		Crippen Method
mcvol	193.310	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
tb	757.41	K	Joback Method
tc	986.09	K	Joback Method
tf	524.76	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.97	J/mol×K	947.97	Joback Method
cpg	539.51	J/mol×K	757.41	Joback Method
cpg	551.26	J/mol×K	795.52	Joback Method
cpg	562.18	J/mol×K	833.64	Joback Method
cpg	572.36	J/mol×K	871.75	Joback Method
cpg	581.92	J/mol×K	909.86	Joback Method
cpg	599.61	J/mol×K	986.09	Joback Method
hsubt	91.00	kJ/mol	323.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7396909&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

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
hsubt:	Enthalpy of sublimation at a given temperature
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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