3-Methylcatechol, bis(trifluoroacetate)

Inchi: InChI=1S/C11H6F6O4/c1-5-3-2-4-6(20-8(18)10(12,13)14)7(5)21-9(19)11(15,16)17/h2-4H
InchiKey: DHLFFAPMPMJESG-UHFFFAOYSA-N
Formula: C11H6F6O4
SMILES: Cc1cccc(OC(=O)C(F)(F)F)c1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 316.15
CAS: 25854-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-1496.13	kJ/mol	Joback Method
hf	-1740.54	kJ/mol	Joback Method
hfus	26.74	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.930		Crippen Method
mcvol	167.590	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
tb	629.46	K	Joback Method
tc	815.20	K	Joback Method
tf	417.89	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.58	J/mol×K	629.46	Joback Method
cpg	451.74	J/mol×K	660.42	Joback Method
cpg	461.19	J/mol×K	691.37	Joback Method
cpg	469.97	J/mol×K	722.33	Joback Method
cpg	478.09	J/mol×K	753.28	Joback Method
cpg	485.59	J/mol×K	784.24	Joback Method
cpg	492.49	J/mol×K	815.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25854506&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