3-Mercaptophenol, O,S-bis(chlorodifluoroacetyl)-

Inchi: InChI=1S/C10H4Cl2F4O3S/c11-9(13,14)7(17)19-5-2-1-3-6(4-5)20-8(18)10(12,15)16/h1-4

InchiKey: REVIVWSKBUVZLP-UHFFFAOYSA-N

Formula: C10H4Cl2F4O3S

SMILES: O=C(Oc1cccc(SC(=O)C(F)(F)Cl)c1)C(F)(F)Cl

Mol. weight [g/mol]: 351.10

Physical Properties

Property code	Value	Unit	Source
gf	-991.04	kJ/mol	Joback Method
hf	-1173.60	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	66.42	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.874		Crippen Method
mcvol	184.920	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	724.28	K	Joback Method
tc	952.56	K	Joback Method
tf	464.93	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.44	J/mol×K	724.28	Joback Method
cpg	451.54	J/mol×K	762.33	Joback Method
cpg	458.75	J/mol×K	800.37	Joback Method
cpg	465.14	J/mol×K	838.42	Joback Method
cpg	470.76	J/mol×K	876.47	Joback Method
cpg	475.69	J/mol×K	914.51	Joback Method
cpg	479.99	J/mol×K	952.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376277&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