1,4-Benzenedithiol, S,S'-bis(chlorodifluoroacetyl)-

Inchi: InChI=1S/C10H4Cl2F4O2S2/c11-9(13,14)7(17)19-5-1-2-6(4-3-5)20-8(18)10(12,15)16/h1
InchiKey: QLEUVHCDAGEPOU-UHFFFAOYSA-N
Formula: C10H4Cl2F4O2S2
SMILES: O=C(Sc1ccc(SC(=O)C(F)(F)Cl)cc1)C(F)(F)Cl
Mol. weight [g/mol]: 367.17

Physical Properties

Property code	Value	Unit	Source
gf	-852.92	kJ/mol	Joback Method
hf	-999.51	kJ/mol	Joback Method
hfus	32.65	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.587		Crippen Method
mcvol	195.400	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook
tb	770.64	K	Joback Method
tc	1016.68	K	Joback Method
tf	477.10	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.07	J/mol×K	770.64	Joback Method
cpg	469.47	J/mol×K	811.65	Joback Method
cpg	475.92	J/mol×K	852.65	Joback Method
cpg	481.51	J/mol×K	893.66	Joback Method
cpg	486.33	J/mol×K	934.66	Joback Method
cpg	490.47	J/mol×K	975.67	Joback Method
cpg	494.03	J/mol×K	1016.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376247&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