1,4-Benzenedithiol, S-chlorodifluoroacetyl-S'-trifluoroacetyl-

Inchi: InChI=1S/C10H4ClF5O2S2/c11-9(12,13)7(17)19-5-1-3-6(4-2-5)20-8(18)10(14,15)16/h1-4

InchiKey: AUKXPFQLLSQIQO-UHFFFAOYSA-N

Formula: C10H4ClF5O2S2

SMILES: O=C(Sc1ccc(SC(=O)C(F)(F)Cl)cc1)C(F)(F)F

Mol. weight [g/mol]: 350.71

Physical Properties

Property code	Value	Unit	Source
gf	-1035.80	kJ/mol	Joback Method
hf	-1179.88	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	65.63	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.318		Crippen Method
mcvol	184.930	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	732.48	K	Joback Method
tc	965.96	K	Joback Method
tf	447.77	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.92	J/mol×K	732.48	Joback Method
cpg	460.09	J/mol×K	771.39	Joback Method
cpg	467.31	J/mol×K	810.31	Joback Method
cpg	473.66	J/mol×K	849.22	Joback Method
cpg	479.22	J/mol×K	888.13	Joback Method
cpg	484.05	J/mol×K	927.05	Joback Method
cpg	488.25	J/mol×K	965.96	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=U376248&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