

1,3-Benzenedithiol, S,S'-bis(chlorodifluoroacetyl)-

Inchi:	InChI=1S/C10H4Cl2F4O2S2/c11-9(13,14)7(17)19-5-2-1-3-6(4-5)20-8(18)10(12,15)16/h1
InchiKey:	FZHFMHLYLBOZQQ-UHFFFAOYSA-N
Formula:	C10H4Cl2F4O2S2
SMILES:	O=C(Sc1cccc(SC(=O)C(F)(F)Cl)c1)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
mvol	195.400	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	770.64	K	Joback Method
tc	1016.68	K	Joback Method
tf	477.10	K	Joback Method
vc	0.755	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U376245&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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