

Catechol, bis(chlorodifluoroacetate)

Inchi:	InChI=1S/C10H4Cl2F4O4/c11-9(13,14)7(17)19-5-3-1-2-4-6(5)20-8(18)10(12,15)16/h1-4H
InchiKey:	NIHDWTRUAWNQLQY-UHFFFAOYSA-N
Formula:	C10H4Cl2F4O4
SMILES:	O=C(Oc1ccccc1OC(=O)C(F)(F)Cl)C(F)(F)Cl
Mol. weight [g/mol]:	335.04

Physical Properties

Property code	Value	Unit	Source
gf	-1129.16	kJ/mol	Joback Method
hf	-1347.69	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.161		Crippen Method
mcvol	174.440	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
rinpola	1321.00		NIST Webbook
rinpola	1321.00		NIST Webbook
tb	677.92	K	Joback Method
tc	888.89	K	Joback Method
tf	452.76	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.20	J/molxK	677.92	Joback Method
cpg	431.85	J/molxK	713.08	Joback Method
cpg	439.70	J/molxK	748.24	Joback Method
cpg	446.80	J/molxK	783.41	Joback Method
cpg	453.18	J/molxK	818.57	Joback Method
cpg	458.90	J/molxK	853.73	Joback Method
cpg	463.99	J/molxK	888.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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