Hydroquinone, chlorodifluoroacetate, trifluoroacetate

Inchi: InChI=1S/C10H4ClF5O4/c11-9(12,13)7(17)19-5-1-3-6(4-2-5)20-8(18)10(14,15)16/h1-4H

InchiKey: RACLHIAQJREFCN-UHFFFAOYSA-N

Formula: C10H4ClF5O4

SMILES: O=C(Oc1ccc(OC(=O)C(F)(F)Cl)cc1)C(F)(F)F

Mol. weight [g/mol]: 318.58

Physical Properties

Property code	Value	Unit	Source
gf	-1312.04	kJ/mol	Joback Method
hf	-1528.06	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.891		Crippen Method
mcvol	163.970	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
tb	639.76	K	Joback Method
tc	838.55	K	Joback Method
tf	423.43	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.01	J/mol×K	639.76	Joback Method
cpg	419.24	J/mol×K	672.89	Joback Method
cpg	427.71	J/mol×K	706.02	Joback Method
cpg	435.45	J/mol×K	739.16	Joback Method
cpg	442.51	J/mol×K	772.29	Joback Method
cpg	448.92	J/mol×K	805.42	Joback Method
cpg	454.71	J/mol×K	838.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376233&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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