

Hydrocinnamic acid, 4-(4-hydroxy-3-iodophenoxy)-3,5-diiodo-

Inchi:	InChI=1S/C15H11I3O4/c16-10-7-9(2-3-13(10)19)22-15-11(17)5-8(6-12(15)18)1-4-14(20)
InchiKey:	VRORTNGXAKZJML-UHFFFAOYSA-N
Formula:	C15H11I3O4
SMILES:	O=C(O)CCc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1
Mol. weight [g/mol]:	635.96
CAS:	51-26-3

Physical Properties

Property code	Value	Unit	Source
gf	-89.28	kJ/mol	Joback Method
hf	-269.48	kJ/mol	Joback Method
hfus	47.01	kJ/mol	Joback Method
hvap	123.15	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.016		Crippen Method
mcvol	271.330	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	1144.39	K	Joback Method
tc	1430.79	K	Joback Method
tf	780.61	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.72	J/molxK	1144.39	Joback Method
cpg	718.71	J/molxK	1383.06	Joback Method
cpg	703.34	J/molxK	1335.33	Joback Method
cpg	689.26	J/molxK	1287.59	Joback Method
cpg	676.27	J/molxK	1239.86	Joback Method
cpg	664.16	J/molxK	1192.12	Joback Method
cpg	735.59	J/molxK	1430.79	Joback Method
dvisc	0.0000001	Paxs	1144.39	Joback Method
dvisc	0.0000002	Paxs	1083.76	Joback Method

dvisc	0.0000003	Paxs	1023.13	Joback Method
dvisc	0.0000005	Paxs	962.50	Joback Method
dvisc	0.0000008	Paxs	901.87	Joback Method
dvisc	0.0000015	Paxs	841.24	Joback Method
dvisc	0.0000029	Paxs	780.61	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=C51263&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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