

Alanine, (3,5-diiodo-4-(-p-hydroxyphenoxy)phenyl)-

Inchi:	InChI=1S/C15H13I2NO4/c16-11-5-8(7-13(18)15(20)21)6-12(17)14(11)22-10-3-1-9(19)2-
InchiKey:	ZHSOTLOTDDYIIK-UHFFFAOYSA-N
Formula:	C15H13I2NO4
SMILES:	NC(Cc1cc(I)c(Oc2ccc(O)cc2)c(I)c1)C(=O)O
Mol. weight [g/mol]:	525.08
CAS:	534-51-0

Physical Properties

Property code	Value	Unit	Source
gf	-73.76	kJ/mol	Joback Method
hf	-306.37	kJ/mol	Joback Method
hfus	44.66	kJ/mol	Joback Method
hvap	123.37	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.348		Crippen Method
mcvol	255.490	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	1118.36	K	Joback Method
tc	1394.35	K	Joback Method
tf	778.29	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.64	J/molxK	1118.36	Joback Method
cpg	688.26	J/molxK	1164.36	Joback Method
cpg	699.18	J/molxK	1210.36	Joback Method
cpg	710.59	J/molxK	1256.35	Joback Method
cpg	722.68	J/molxK	1302.35	Joback Method
cpg	735.63	J/molxK	1348.35	Joback Method
cpg	749.62	J/molxK	1394.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C534510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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