Propanoic acid, 2-amino,3-[3,5-diiodo-4-[4-hydroxy-3-(1-methyleth

Inchi: InChI=1S/C18H19I2NO4/c1-9(2)12-8-11(3-4-16(12)22)25-17-13(19)5-10(6-14(17)20)7-15

InchiKey: RNNRJYLAQGIPJH-UHFFFAOYSA-N

Formula: C18H19I2NO4

SMILES: CC(C)c1cc(Oc2c(I)cc(CC(N)C(=O)O)cc2I)ccc1O

Mol. weight [g/mol]: 567.16

CAS: 10439-94-8

Physical Properties

Property code	Value	Unit	Source
gf	-60.57	kJ/mol	Joback Method
hf	-385.04	kJ/mol	Joback Method
hfus	48.52	kJ/mol	Joback Method
hvap	130.32	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.472		Crippen Method
mcvol	297.760	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	1191.54	K	Joback Method
tc	1467.76	K	Joback Method
tf	809.62	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.68	J/mol×K	1191.54	Joback Method
cpg	869.52	J/mol×K	1237.58	Joback Method
cpg	882.71	J/mol×K	1283.61	Joback Method
cpg	896.42	J/mol×K	1329.65	Joback Method
cpg	910.86	J/mol×K	1375.69	Joback Method
cpg	926.21	J/mol×K	1421.72	Joback Method
cpg	942.66	J/mol×K	1467.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10439948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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