Benzamide, 2-amino-3,5-diiodo-

Inchi: InChI=1S/C7H6I2N2O/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2H,10H2,(H2,11,12)
InchiKey: WDDCFATZFHRUQL-UHFFFAOYSA-N
Formula: C7H6I2N2O
SMILES: NC(=O)c1cc(I)cc(I)c1N
Mol. weight [g/mol]: 387.94

Physical Properties

Property code	Value	Unit	Source
gf	211.80	kJ/mol	Joback Method
hf	123.05	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	1.577		Crippen Method
mcvol	158.900	ml/mol	McGowan Method
pc	4621.41	kPa	Joback Method
tb	786.39	K	Joback Method
tc	1089.92	K	Joback Method
tf	565.20	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.20	J/mol×K	786.39	Joback Method
cpg	314.05	J/mol×K	836.98	Joback Method
cpg	320.24	J/mol×K	887.57	Joback Method
cpg	325.87	J/mol×K	938.16	Joback Method
cpg	331.03	J/mol×K	988.74	Joback Method
cpg	335.80	J/mol×K	1039.33	Joback Method
cpg	340.28	J/mol×K	1089.92	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=B6010383&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume