Diatrizoic acid

Inchi: InChI=1S/C11H9I3N2O4/c1-3(17)15-9-6(12)5(11(19)20)7(13)10(8(9)14)16-4(2)18/h1-2H
InchiKey: YVPYQUNUQOZFHG-UHFFFAOYSA-N
Formula: C11H9I3N2O4
SMILES: CC(=O)Nc1c(I)c(NC(C)=O)c(I)c(C(=O)O)c1I
Mol. weight [g/mol]: 613.92

Physical Properties

Property code	Value	Unit	Source
gf	-64.44	kJ/mol	Joback Method
hf	-243.61	kJ/mol	Joback Method
hfus	48.64	kJ/mol	Joback Method
hvap	123.57	kJ/mol	Joback Method
log10ws	-2.01		Aqueous Solubility Prediction Method
log10ws	-2.79		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.115		Crippen Method
mcvol	250.090	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	1136.21	K	Joback Method
tc	1408.63	K	Joback Method
tf	792.86	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.26	J/mol×K	1136.21	Joback Method
cpg	563.41	J/mol×K	1181.61	Joback Method
cpg	568.25	J/mol×K	1227.02	Joback Method
cpg	572.87	J/mol×K	1272.42	Joback Method
cpg	577.33	J/mol×K	1317.82	Joback Method
cpg	581.72	J/mol×K	1363.23	Joback Method
cpg	586.13	J/mol×K	1408.63	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
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