2-methyl-3,5-dinitrobenzoic acid

Inchi: InChI=1S/C8H6N2O6/c1-4-6(8(11)12)2-5(9(13)14)3-7(4)10(15)16/h2-3H,1H3,(H,11,12)
InchiKey: CDVNZMKTJIBBBV-UHFFFAOYSA-N
Formula: C8H6N2O6
SMILES: Cc1c(C(=O)O)cc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 226.14

Physical Properties

Property code	Value	Unit	Source
gf	-94.64	kJ/mol	Joback Method
hf	-292.66	kJ/mol	Joback Method
hfus	37.76	kJ/mol	Joback Method
hvap	94.27	kJ/mol	Joback Method
log10ws	-2.60		Aqueous Solubility Prediction Method
logp	1.510		Crippen Method
mcvol	142.100	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
tb	873.79	K	Joback Method
tc	1122.17	K	Joback Method
tf	641.87	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.75	J/mol×K	873.79	Joback Method
cpg	393.29	J/mol×K	915.19	Joback Method
cpg	399.14	J/mol×K	956.58	Joback Method
cpg	404.32	J/mol×K	997.98	Joback Method
cpg	408.87	J/mol×K	1039.37	Joback Method
cpg	412.82	J/mol×K	1080.77	Joback Method
cpg	416.20	J/mol×K	1122.17	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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