2-DIBENZOFURANSULFONIC ACID

Other names: Dibenzofuran-2-sulphonic acid
dibenzofuran-2-sulfonic acid
Inchi: InChI=1S/C12H8O4S/c13-17(14,15)8-5-6-12-10(7-8)9-3-1-2-4-11(9)16-12/h1-7H,(H,13,1
InchiKey: JANFYPHFIPGYTQ-UHFFFAOYSA-N
Formula: C12H8O4S
SMILES: O=S(=O)(O)c1ccc2oc3ccccc3c2c1
Mol. weight [g/mol]: 248.26

Physical Properties

Property code	Value	Unit	Source
hf	-448.45	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-0.47		Aqueous Solubility Prediction Method
logp	2.833		Crippen Method
mcvol	161.390	ml/mol	McGowan Method
pc	3108.78	kPa	Cheméo Relay (1.0, beta)
tb	678.04	K	Cheméo Relay (1.0)
tc	1011.88	K	Cheméo Relay (1.0)
tf	553.01	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83863632&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
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