

naphthalene-2-sulfonic acid

Inchi:

lnchl=1S/C10H8O3S/c11-14(12,13)10-6-5-8-3-1-2-4-9(8)7-10/h1-7H,(H,11,12,13)

InchiKey:

KVBGVZZKJNLNJU-UHFFFAOYSA-N

Formula:

C10H8O3S

SMILES:

O=S(=O)(O)c1ccc2ccccc2c1

Mol. weight [g/mol]:

208.24

Physical Properties

Property code	Value	Unit	Source
gf	-362.61	kJ/mol	Joback Method
hf	-439.18	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	77.75	kJ/mol	Joback Method
log10ws	-1.26		Aqueous Solubility Prediction Method
logp	2.087		Crippen Method
mcvol	142.500	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
tb	618.80	K	Joback Method
tc	830.39	K	Joback Method
tf	373.48	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.29	J/mol×K	618.80	Joback Method
cpg	343.83	J/mol×K	654.06	Joback Method
cpg	353.58	J/mol×K	689.33	Joback Method
cpg	362.58	J/mol×K	724.59	Joback Method
cpg	370.85	J/mol×K	759.86	Joback Method
cpg	378.43	J/mol×K	795.12	Joback Method
cpg	385.37	J/mol×K	830.39	Joback Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

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