N-naphthalen-2-yl-2-sulfanylacetamide

Inchi: InChI=1S/C12H11NOS/c14-12(8-15)13-11-6-5-9-3-1-2-4-10(9)7-11/h1-7,15H,8H2,(H,13,

InchiKey: SGMHGVVTMOGJMX-UHFFFAOYSA-N

Formula: C12H11NOS

SMILES: O=C(CS)Nc1ccc2ccccc2c1

Mol. weight [g/mol]: 217.29

Physical Properties

Property code	Value	Unit	Source
gf	249.45	kJ/mol	Joback Method
hf	104.49	kJ/mol	Joback Method
hfus	28.25	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-3.34		Aqueous Solubility Prediction Method
logp	2.708		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	691.50	K	Joback Method
tc	945.79	K	Joback Method
tf	384.65	K	Aqueous Solubility Prediction Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.70	J/mol×K	691.50	Joback Method
cpg	418.34	J/mol×K	733.88	Joback Method
cpg	429.91	J/mol×K	776.26	Joback Method
cpg	440.51	J/mol×K	818.65	Joback Method
cpg	450.25	J/mol×K	861.03	Joback Method
cpg	459.22	J/mol×K	903.41	Joback Method
cpg	467.53	J/mol×K	945.79	Joback Method

Sources

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
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