Naphthalene, 1,4-bis(methylthio)-

Inchi: InChI=1S/C12H12S2/c1-13-11-7-8-12(14-2)10-6-4-3-5-9(10)11/h3-8H,1-2H3
InchiKey: ZYYGYYVWYHXYOF-UHFFFAOYSA-N
Formula: C12H12S2
SMILES: CSc1ccc(SC)c2ccccc12
Mol. weight [g/mol]: 220.35
CAS: 10075-73-7

Physical Properties

Property code	Value	Unit	Source
gf	316.20	kJ/mol	Joback Method
hf	197.39	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
ie	7.58	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
log10ws	-4.76		Crippen Method
logp	4.284		Crippen Method
mcvol	169.420	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	667.14	K	Joback Method
tc	937.30	K	Joback Method
tf	377.96	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.87	J/mol×K	667.14	Joback Method
cpg	410.18	J/mol×K	712.17	Joback Method
cpg	423.28	J/mol×K	757.19	Joback Method
cpg	435.25	J/mol×K	802.22	Joback Method
cpg	446.15	J/mol×K	847.25	Joback Method
cpg	456.07	J/mol×K	892.28	Joback Method
cpg	465.07	J/mol×K	937.30	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10075737&Units=SI
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
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
vc:	Critical Volume