Naphthalene-1,8-disulfide-S-oxide

Inchi: InChI=1S/C10H6OS2/c11-13-9-6-2-4-7-3-1-5-8(12-13)10(7)9/h1-6H
InchiKey: LIRFRPDBUURHNY-UHFFFAOYSA-N
Formula: C10H6OS2
SMILES: O=S1Sc2cccc3cccc1c23
Mol. weight [g/mol]: 206.28
CAS: 49833-12-7

Physical Properties

Property code	Value	Unit	Source
gf	142.57	kJ/mol	Joback Method
hf	97.14	kJ/mol	Joback Method
hfus	22.04	kJ/mol	Joback Method
hvap	60.68	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.968		Crippen Method
mcvol	136.250	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
tb	576.12	K	Joback Method
tc	836.60	K	Joback Method
tf	481.30	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.00	J/mol×K	576.12	Joback Method
cpg	299.11	J/mol×K	619.53	Joback Method
cpg	309.08	J/mol×K	662.95	Joback Method
cpg	318.06	J/mol×K	706.36	Joback Method
cpg	326.22	J/mol×K	749.78	Joback Method
cpg	333.71	J/mol×K	793.19	Joback Method
cpg	340.69	J/mol×K	836.60	Joback Method

Sources

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=C49833127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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