2-Mercapto-1,4-naphthoquinone

Inchi: InChI=1S/C10H6O2S/c11-8-5-9(13)10(12)7-4-2-1-3-6(7)8/h1-5,13H
InchiKey: RWSGVVRLMWVPTI-UHFFFAOYSA-N
Formula: C10H6O2S
SMILES: O=C1C=C(S)C(=O)c2ccccc21
Mol. weight [g/mol]: 190.22
CAS: 116401-72-0

Physical Properties

Property code	Value	Unit	Source
gf	-3.00	kJ/mol	Joback Method
hf	-128.30	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	57.37	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	1.879		Crippen Method
mcvol	132.330	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	678.18	K	Joback Method
tc	965.95	K	Joback Method
tf	446.24	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.11	J/mol×K	678.18	Joback Method
cpg	326.07	J/mol×K	726.14	Joback Method
cpg	337.91	J/mol×K	774.10	Joback Method
cpg	348.59	J/mol×K	822.06	Joback Method
cpg	358.11	J/mol×K	870.02	Joback Method
cpg	366.43	J/mol×K	917.99	Joback Method
cpg	373.53	J/mol×K	965.95	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=C116401720&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