

1,1'-Dithiodi-2-naphthol

Inchi:	InChI=1S/C20H14O2S2/c21-17-11-9-13-5-1-3-7-15(13)19(17)23-24-20-16-8-4-2-6-14(16)
InchiKey:	RFAXLXKIAKIUDT-UHFFFAOYSA-N
Formula:	C20H14O2S2
SMILES:	Oc1ccc2ccccc2c1SSc1c(O)ccc2ccccc12
Mol. weight [g/mol]:	350.45
CAS:	42521-82-4

Physical Properties

Property code	Value	Unit	Source
gf	293.38	kJ/mol	Joback Method
hf	105.25	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	108.93	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.204		Crippen Method
mcvol	250.660	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	1057.08	K	Joback Method
tc	1359.34	K	Joback Method
tf	750.68	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.45	J/molxK	1057.08	Joback Method
cpg	761.31	J/molxK	1107.46	Joback Method
cpg	780.69	J/molxK	1157.83	Joback Method
cpg	802.05	J/molxK	1208.21	Joback Method
cpg	825.85	J/molxK	1258.59	Joback Method
cpg	852.55	J/molxK	1308.96	Joback Method
cpg	882.61	J/molxK	1359.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C42521824&Units=SI

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
mccvol:	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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