

Naphtho[1,8-cd]-1,2-dithiole

Other names:	1,2-Dithiaacenaphthene 1,8-Naphthylene disulfide
Inchi:	InChI=1S/C10H6S2/c1-3-7-4-2-6-9-10(7)8(5-1)11-12-9/h1-6H
InchiKey:	NDOFGUDEKQECDN-UHFFFAOYSA-N
Formula:	C10H6S2
SMILES:	<chem>c1cc2c3c(cccc3c1)SS2</chem>
Mol. weight [g/mol]:	190.28
CAS:	209-22-3

Physical Properties

Property code	Value	Unit	Source
gf	393.40	kJ/mol	Joback Method
hf	344.75	kJ/mol	Joback Method
hfus	18.42	kJ/mol	Joback Method
hvap	54.77	kJ/mol	Joback Method
ie	7.14	eV	NIST Webbook
ie	7.10	eV	NIST Webbook
ie	7.10	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
log10ws	-4.81		Crippen Method
logp	3.953		Crippen Method
mcvol	130.380	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	586.62	K	Joback Method
tc	864.97	K	Joback Method
tf	389.70 ± 0.50	K	NIST Webbook
vc	0.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.71	J/mol×K	586.62	Joback Method
cpg	282.52	J/mol×K	633.01	Joback Method
cpg	292.17	J/mol×K	679.40	Joback Method

cpg	300.87	J/mol×K	725.79	Joback Method
cpg	308.83	J/mol×K	772.18	Joback Method
cpg	316.23	J/mol×K	818.58	Joback Method
cpg	323.30	J/mol×K	864.97	Joback Method
hfust	13.00	kJ/mol	394.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C209223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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

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