

Di-«beta»-naphthyl disulfide

Other names:

Di-2-Naphthyl disulfide
Disulfide, di-2-naphthalenyl
2-Naphthyl disulfide
«beta», «beta»-Dinaphthyldisulfid

Inchi:

InChI=1S/C20H14S2/c1-3-7-17-13-19(11-9-15(17)5-1)21-22-20-12-10-16-6-2-4-8-18(16)

InchiKey:

SUPMWVVVBKKGEL-UHFFFAOYSA-N

Formula:

C20H14S2

SMILES:

c1ccc2cc(SSc3ccc4ccccc4c3)ccc2c1

Mol. weight [g/mol]:

318.45

CAS:

5586-15-2

Physical Properties

Property code	Value	Unit	Source
gf	602.62	kJ/mol	Joback Method
hf	459.87	kJ/mol	Joback Method
hfus	37.16	kJ/mol	Joback Method
hvap	82.90	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.792		Crippen Method
mcvol	238.920	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
tb	895.84	K	Joback Method
tc	1194.15	K	Joback Method
tf	527.24	K	Joback Method
vc	0.891	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.06	J/mol×K	895.84	Joback Method
cpg	665.85	J/mol×K	945.56	Joback Method
cpg	678.48	J/mol×K	995.28	Joback Method
cpg	690.20	J/mol×K	1044.99	Joback Method
cpg	701.24	J/mol×K	1094.71	Joback Method

cpg	711.86	J/mol×K	1144.43	Joback Method
cpg	722.31	J/mol×K	1194.15	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=C5586152&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

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