

.beta.,.beta.-Dinaphthylidisulfid

Other names:	2-Naphthyl disulfide Di-2-Naphthyl disulfide Disulfide, di-2-naphthalenyl «beta»,«beta»-Dinaphthylidisulfid
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]:	318.47

Physical Properties

Property code	Value	Unit	Source
af	0.5224		Cheméo Relay (1.0)
gf	602.62	kJ/mol	Joback Method
hf	378.57	kJ/mol	Cheméo Relay (1.0)
hfus	37.16	kJ/mol	Joback Method
hvap	127.57	kJ/mol	Cheméo Relay (1.0)
ie	7.54	eV	Cheméo Relay (1.0)
log10ws	-8.76		Cheméo Relay (1.0)
logp	6.792		Crippen Method
mcvol	238.920	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
tb	756.27	K	Cheméo Relay (1.0)
tc	1056.09	K	Cheméo Relay (1.0)
tf	470.59	K	Cheméo Relay (1.0)
vc	0.861	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5586152&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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