

4,4'-DIAMINODIPHENYLSULPHOXIDE

Other names:	4,4'-Diaminodiphenyl sulfoxide 4,4'-Diaminodiphenylsulphoxide 4,4'-Diaminophenyl sulfoxide 4,4'-Sulfinyldianiline Aniline, 4,4'-sulfinyldi- Aniline, p,p'-sulfinyldi- Benzenamine, 4,4'-sulfinylbis- Bis(p-aminophenyl) sulfoxide DDSO Di(p-aminophenyl) sulfoxide Medapsol NSC 6090 p,p'-Diaminodiphenyl sulphoxide p,p'-Sulfinyldianiline
Inchi:	InChI=1S/C12H12N2OS/c13-9-1-5-11(6-2-9)16(15)12-7-3-10(14)4-8-12/h1-8H,13-14H2
InchiKey:	MITHMOYLTXMLRB-UHFFFAOYSA-N
Formula:	C12H12N2OS
SMILES:	Nc1ccc(S(=O)c2ccc(N)cc2)cc1
Mol. weight [g/mol]:	232.31

Physical Properties

Property code	Value	Unit	Source
hf	84.06	kJ/mol	Cheméo Relay (1.0)
hfus	32.29	kJ/mol	Joback Method
ie	7.34	eV	Cheméo Relay (1.0)
log10ws	-3.08		Cheméo Relay (1.0)
logp	2.018		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
tb	685.94	K	Cheméo Relay (1.0)
tf	434.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	456.49	J/mol×K	740.62	Joback Method
cpg	469.52	J/mol×K	784.98	Joback Method
cpg	481.24	J/mol×K	829.34	Joback Method
cpg	491.71	J/mol×K	873.70	Joback Method
cpg	500.98	J/mol×K	918.05	Joback Method
cpg	509.10	J/mol×K	962.41	Joback Method
cpg	516.15	J/mol×K	1006.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119595&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
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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