

Methanethione, bis[4-(dimethylamino)phenyl]-

Other names:

Benzophenone, 4,4'-bis(dimethylamino)thio-
p,p'-bis(Dimethylamino)thiobenzophenone
Michler's thioketone
Michler's thione
4,4'-Bis(dimethylamino)thiobenzophenone
p,p'-Tetramethyldiaminothiobenzophenone
Bis[4-(dimethylamino)phenyl]methanethione
NSC 30656

Inchi:

InChI=1S/C17H20N2S/c1-18(2)15-9-5-13(6-10-15)17(20)14-7-11-16(12-8-14)19(3)4/h5-1

InchiKey:

KFUJUTFTRXYQMG-UHFFFAOYSA-N

Formula:

C17H20N2S

SMILES:

CN(C)c1ccc(C(=S)c2ccc(N(C)C)cc2)cc1

Mol. weight [g/mol]:

284.42

CAS:

1226-46-6

Physical Properties

Property code	Value	Unit	Source
gf	636.44	kJ/mol	Joback Method
hf	337.47	kJ/mol	Joback Method
hfus	37.73	kJ/mol	Joback Method
hvap	70.13	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.585		Crippen Method
mcvol	234.880	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
tb	746.60	K	Joback Method
tc	987.12	K	Joback Method
tf	458.44	K	Joback Method
vc	0.844	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.27	J/mol×K	746.60	Joback Method

cpg	652.91	J/mol×K	786.69	Joback Method
cpg	668.32	J/mol×K	826.77	Joback Method
cpg	682.64	J/mol×K	866.86	Joback Method
cpg	696.01	J/mol×K	906.95	Joback Method
cpg	708.58	J/mol×K	947.04	Joback Method
cpg	720.49	J/mol×K	987.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1226466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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