

2,6,2',6'-TETRAMETHYLAZOBENZENE

Other names:	2,2',6,6'-Tetramethylazobenzene-N,N-dioxide
Inchi:	InChI=1S/C16H18N2O2/c1-11-7-5-8-12(2)15(11)17(19)18(20)16-13(3)9-6-10-14(16)4/h5
InchiKey:	MOIONWYNTORJQI-UHFFFAOYSA-N
Formula:	C16H18N2O2
SMILES:	Cc1cccc(C)c1[N+](=[O-])=[N+](=[O-])c1c(C)cccc1C
Mol. weight [g/mol]:	270.33

Physical Properties

Property code	Value	Unit	Source
af	0.6618		Cheméo Relay (1.0)
gf	483.50	kJ/mol	Cheméo Relay (1.0, beta)
hf	203.42	kJ/mol	Cheméo Relay (1.0)
hsub	107.00 ± 12.00	kJ/mol	NIST Webbook
hvap	90.33	kJ/mol	Cheméo Relay (1.0)
ie	7.93	eV	Cheméo Relay (1.0)
log10ws	-4.95		Cheméo Relay (1.0)
logp	4.356		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2001.99	kPa	Cheméo Relay (1.0, beta)
tb	597.21	K	Cheméo Relay (1.0)
tc	910.75	K	Cheméo Relay (1.0)
tf	371.10	K	Cheméo Relay (1.0)
vc	0.752	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101225698&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation 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
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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