

3,7-Diphenyl-5-(p-dimethylaminophenyl)-1,2-diazepine

Other names:	3,7-Diphenyl-5-(p-dimethylaminophenyl)-1,2(4H)-diazepine
Inchi:	InChI=1S/C25H23N3/c1-28(2)23-15-13-19(14-16-23)22-17-24(20-9-5-3-6-10-20)26-27-2
InchiKey:	VXVJBLRSHSQLAK-UHFFFAOYSA-N
Formula:	C25H23N3
SMILES:	CN(C)c1ccc(C2=CC(c3ccccc3)=NN=C(c3ccccc3)C2)cc1
Mol. weight [g/mol]:	365.47
CAS:	32059-53-3

Physical Properties

Property code	Value	Unit	Source
gf	912.61	kJ/mol	Joback Method
hf	555.69	kJ/mol	Joback Method
hfus	46.70	kJ/mol	Joback Method
hvap	96.97	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.433		Crippen Method
mcvol	298.010	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
tb	1017.17	K	Joback Method
tc	1301.19	K	Joback Method
tf	686.78	K	Joback Method
vc	1.111	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.16	J/molxK	1017.17	Joback Method
cpg	992.75	J/molxK	1064.51	Joback Method
cpg	1002.92	J/molxK	1111.84	Joback Method
cpg	1010.80	J/molxK	1159.18	Joback Method
cpg	1016.51	J/molxK	1206.51	Joback Method
cpg	1020.19	J/molxK	1253.85	Joback Method
cpg	1021.95	J/molxK	1301.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32059533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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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