

4-(4-Diethylamino-2-methylphenylimino)-1-oxo-N-

Other names:	2-Phenylcarbamoyl-1,4-naphthoquinone-4-(4-diethylamino-2-methylphenyl)imine 2-Naphthanilide, 4-[4-diethylamino-o-tolylimino]-1,4-dihydro-1-oxo-
Inchi:	InChI=1S/C28H27N3O2/c1-4-31(5-2)21-15-16-25(19(3)17-21)30-26-18-24(27(32)23-14-
InchiKey:	ZYKBEIDPRRYKKQ-UHFFFAOYSA-N
Formula:	C28H27N3O2
SMILES:	CCN(CC)c1ccc(N=C2C=C(C(=O)Nc3ccccc3)C(=O)c3ccccc32)c(C)c1
Mol. weight [g/mol]:	437.53
CAS:	102187-19-9

Physical Properties

Property code	Value	Unit	Source
hf	98.97	kJ/mol	Joback Method
hvap	111.70	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.723		Crippen Method
mcvol	347.720	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
tb	1218.30	K	Joback Method
tc	1494.94	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102187199&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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