

Indoaniline dye, [1-hydroxy-2-(2,4,6-trimethyl)naphthanilide with 4-amino-n,n-diethyl-3-methylaniline]

InChI: CCN(CC)c1ccc(N=C2C=C(C(=O)Nc3c(C)cc(C)cc3C)C(=O)c3ccccc32)c(C)c1
InChIKey: QDWGEPBQPKLIGJ-VEVQFJJOQSA-N

Formula: C₃₁H₃₃N₃O₂
SMILES: CCN(CC)c1ccc(N=C2C=C(C(=O)Nc3c(C)cc(C)cc3C)C(=O)c3ccccc32)c(C)c1
Mol. weight [g/mol]: 479.61
CAS: 114909-96-5

Physical Properties

Property code	Value	Unit	Source
hf	2.64	kJ/mol	Joback Method
hvap	120.36	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	6.649		Crippen Method
mcvol	389.990	ml/mol	McGowan Method
pc	1039.91	kPa	Joback Method
tb	1301.88	K	Joback Method
tc	1594.46	K	Joback Method

Sources

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=C114909965&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hf: Enthalpy of formation 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

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