

N,N-Dimethyl-N'-heptyl-p-chlorobenzamide

Inchi: InChI=1S/C16H25ClN2/c1-4-5-6-7-8-13-18-16(19(2)3)14-9-11-15(17)12-10-14/h9-12H,4-
InchiKey: WKAAKJDZAYDGJF-UHFFFAOYSA-N
Formula: C16H25ClN2
SMILES: CCCCCCN=C(c1ccc(Cl)cc1)N(C)C
Mol. weight [g/mol]: 280.84

Physical Properties

Property code	Value	Unit	Source
hf	-24.29	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.619		Crippen Method
mcvol	240.440	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	723.57	K	Joback Method
tc	931.85	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R159227&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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