

Benzamide, 3-methyl-N-decyl-

Inchi: InChI=1S/C18H29NO/c1-3-4-5-6-7-8-9-10-14-19-18(20)17-13-11-12-16(2)15-17/h11-13,
InchiKey: KHDYZFWOHDG NR-UHFFFAOYSA-N
Formula: C18H29NO
SMILES: CCCCCCCCCCN=C(O)c1cccc(C)c1
Mol. weight [g/mol]: 275.43

Physical Properties

Property code	Value	Unit	Source
hf	-269.59	kJ/mol	Joback Method
hvap	78.67	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.440		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	811.64	K	Joback Method
tc	1009.03	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407420&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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