

Benzamide, 3-chloro-N-hexadecyl-

Inchi:	InChI=1S/C23H38ClNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-25-23(26)21-17-16-18
InchiKey:	PKYDZPWVBOLOKP-UHFFFAOYSA-N
Formula:	C23H38ClNO
SMILES:	CCCCCCCCCCCCCCCCN=C(O)c1cccc(Cl)c1
Mol. weight [g/mol]:	380.01

Physical Properties

Property code	Value	Unit	Source
hf	-388.53	kJ/mol	Joback Method
hvap	94.19	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	8.126		Crippen Method
mcvol	334.960	ml/mol	McGowan Method
pc	1004.62	kPa	Joback Method
rinpol	3113.00		NIST Webbook
rinpol	3113.00		NIST Webbook
tb	963.47	K	Joback Method
tc	1179.56	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=U407986&Units=SI

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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