

Benzamide, 3-chloro-N-octadecyl-

Inchi:	InChI=1S/C25H42ClNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-27-25(28)23-19
InchiKey:	JKLJDVKSCRZZOQ-UHFFFAOYSA-N
Formula:	C25H42ClNO
SMILES:	CCCCCCCCCCCCCCCCCN=C(O)c1cccc(Cl)c1
Mol. weight [g/mol]:	408.06

Physical Properties

Property code	Value	Unit	Source
hf	-429.81	kJ/mol	Joback Method
hvap	98.64	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	8.906		Crippen Method
mcpvol	363.140	ml/mol	McGowan Method
pc	892.67	kPa	Joback Method
rinpol	3321.00		NIST Webbook
rinpol	3321.00		NIST Webbook
tb	1009.23	K	Joback Method
tc	1237.56	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407987&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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