Benzamide, 3-chloro-2-fluoro-N-decyl-

Inchi: InChI=1S/C17H25ClFNO/c1-2-3-4-5-6-7-8-9-13-20-17(21)14-11-10-12-15(18)16(14)19/h
InchiKey: YKFLMZBSNOAGCV-UHFFFAOYSA-N
Formula: C17H25ClFNO
SMILES: CCCCCCCCCCN=C(O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 313.84

Physical Properties

Property code	Value	Unit	Source
hf	-472.27	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.924		Crippen Method
mcvol	252.190	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2394.00		NIST Webbook
rinpol	2394.00		NIST Webbook
tb	830.44	K	Joback Method
tc	1028.76	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=U407829&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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