

Benzamide, 3-trifluoromethyl-2-fluoro-N-octadecyl-

Inchi: InChI=1S/C26H41F4NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-31-25(32)22-19
InchiKey: HZYFJOTTYWVSNU-UHFFFAOYSA-N
Formula: C26H41F4NO
SMILES: CCCCCCCCCCCCCCCCCCN=C(O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 459.60

Physical Properties

Property code	Value	Unit	Source
hf	-1239.37	kJ/mol	Joback Method
hvap	92.58	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	9.411		Crippen Method
mcvol	372.070	ml/mol	McGowan Method
pc	779.38	kPa	Joback Method
rinpol	2945.00		NIST Webbook
rinpol	2945.00		NIST Webbook
tb	993.51	K	Joback Method
tc	1226.63	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=U407715&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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