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

Inchi: InChI=1S/C18H27ClFNO/c1-2-3-4-5-6-7-8-9-10-14-21-18(22)15-12-11-13-16(19)17(15)2
InchiKey: ZTFSZVVGJHCSFT-UHFFFAOYSA-N
Formula: C18H27ClFNO
SMILES: CCCCCCCCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 327.86

Physical Properties

Property code	Value	Unit	Source
gf	-52.44	kJ/mol	Joback Method
hf	-472.22	kJ/mol	Joback Method
hfus	49.61	kJ/mol	Joback Method
hvap	76.01	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.740		Crippen Method
mcvol	266.280	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	788.62	K	Joback Method
tc	983.65	K	Joback Method
tf	477.18	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.35	J/mol×K	788.62	Joback Method
cpg	794.01	J/mol×K	821.13	Joback Method
cpg	808.73	J/mol×K	853.63	Joback Method
cpg	822.57	J/mol×K	886.14	Joback Method
cpg	835.56	J/mol×K	918.64	Joback Method
cpg	847.74	J/mol×K	951.15	Joback Method
cpg	859.15	J/mol×K	983.65	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=U407830&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume