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

Inchi: InChI=1S/C19H29ClFNO/c1-2-3-4-5-6-7-8-9-10-11-15-22-19(23)16-13-12-14-17(20)18(1
InchiKey: BJXVBIKYZALXRZ-UHFFFAOYSA-N
Formula: C19H29ClFNO
SMILES: CCCCCCCCCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 341.89

Physical Properties

Property code	Value	Unit	Source
gf	-44.02	kJ/mol	Joback Method
hf	-492.86	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	78.24	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.130		Crippen Method
mcvol	280.370	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	811.50	K	Joback Method
tc	1006.81	K	Joback Method
tf	488.45	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.19	J/mol×K	811.50	Joback Method
cpg	852.16	J/mol×K	844.05	Joback Method
cpg	867.18	J/mol×K	876.60	Joback Method
cpg	881.29	J/mol×K	909.16	Joback Method
cpg	894.53	J/mol×K	941.71	Joback Method
cpg	906.94	J/mol×K	974.26	Joback Method
cpg	918.57	J/mol×K	1006.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407831&Units=SI
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

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