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

Inchi: InChI=1S/C23H37ClFNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-26-23(27)20-17-16-1
InchiKey: ISBMVGQXSBDCTH-UHFFFAOYSA-N
Formula: C23H37ClFNO
SMILES: CCCCCCCCCCCCCCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 398.00

Physical Properties

Property code	Value	Unit	Source
gf	-10.34	kJ/mol	Joback Method
hf	-575.42	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	87.14	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.690		Crippen Method
mcvol	336.730	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	3032.00		NIST Webbook
rinpol	3032.00		NIST Webbook
tb	903.02	K	Joback Method
tc	1106.63	K	Joback Method
tf	533.53	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.82	J/mol×K	903.02	Joback Method
cpg	1093.18	J/mol×K	936.96	Joback Method
cpg	1109.44	J/mol×K	970.89	Joback Method
cpg	1124.67	J/mol×K	1004.83	Joback Method
cpg	1138.92	J/mol×K	1038.76	Joback Method
cpg	1152.24	J/mol×K	1072.70	Joback Method
cpg	1164.71	J/mol×K	1106.63	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=U407833&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