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

Inchi: InChI=1S/C21H33ClFNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-24-21(25)18-15-14-16-19(2
InchiKey: GSHQDUXVHZMJFI-UHFFFAOYSA-N
Formula: C21H33ClFNO
SMILES: CCCCCCCCCCCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 369.94

Physical Properties

Property code	Value	Unit	Source
gf	-27.18	kJ/mol	Joback Method
hf	-534.14	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	82.69	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.910		Crippen Method
mcvol	308.550	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
tb	857.26	K	Joback Method
tc	1055.17	K	Joback Method
tf	510.99	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.47	J/mol×K	857.26	Joback Method
cpg	971.10	J/mol×K	890.25	Joback Method
cpg	986.71	J/mol×K	923.23	Joback Method
cpg	1001.35	J/mol×K	956.22	Joback Method
cpg	1015.08	J/mol×K	989.20	Joback Method
cpg	1027.94	J/mol×K	1022.19	Joback Method
cpg	1039.98	J/mol×K	1055.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407832&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

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