Benzamide, 2-fluoro-3-trifluoromethyl-N-pentyl-N-tetradecyl-

Inchi: InChI=1S/C27H43F4NO/c1-3-5-7-8-9-10-11-12-13-14-15-17-22-32(21-16-6-4-2)26(33)23

InchiKey: COZRBCAXJSAUFH-UHFFFAOYSA-N

Formula: C27H43F4NO

SMILES: CCCCCCCCCCCCCCN(CCCCC)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 473.63

Physical Properties

Property code	Value	Unit	Source
gf	-524.93	kJ/mol	Joback Method
hf	-1225.26	kJ/mol	Joback Method
hfus	68.48	kJ/mol	Joback Method
hvap	83.52	kJ/mol	Joback Method
log10ws	-10.17		Crippen Method
logp	9.178		Crippen Method
mcvol	386.160	ml/mol	McGowan Method
pc	767.76	kPa	Joback Method
tb	913.96	K	Joback Method
tc	1121.19	K	Joback Method
tf	532.69	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1296.30	J/mol×K	913.96	Joback Method
cpg	1316.54	J/mol×K	948.50	Joback Method
cpg	1335.55	J/mol×K	983.04	Joback Method
cpg	1353.45	J/mol×K	1017.58	Joback Method
cpg	1370.33	J/mol×K	1052.12	Joback Method
cpg	1386.30	J/mol×K	1086.66	Joback Method
cpg	1401.45	J/mol×K	1121.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416701&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume