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

Inchi: InChI=1S/C24H37F4NO/c1-3-5-7-8-9-10-11-12-14-19-29(18-13-6-4-2)23(30)20-16-15-17

InchiKey: QZGGMJOWRMXGKM-UHFFFAOYSA-N

Formula: C24H37F4NO

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

Mol. weight [g/mol]: 431.55

Physical Properties

Property code	Value	Unit	Source
gf	-550.19	kJ/mol	Joback Method
hf	-1163.34	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	8.008		Crippen Method
mcvol	343.890	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
tb	845.32	K	Joback Method
tc	1035.24	K	Joback Method
tf	498.88	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.93	J/mol×K	845.32	Joback Method
cpg	1127.39	J/mol×K	876.97	Joback Method
cpg	1144.78	J/mol×K	908.63	Joback Method
cpg	1161.19	J/mol×K	940.28	Joback Method
cpg	1176.68	J/mol×K	971.93	Joback Method
cpg	1191.32	J/mol×K	1003.59	Joback Method
cpg	1205.19	J/mol×K	1035.24	Joback Method

Sources

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=U416699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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