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

Inchi: InChI=1S/C14H17F4NO/c1-3-4-5-9-19(2)13(20)10-7-6-8-11(12(10)15)14(16,17)18/h6-8H

InchiKey: VYENWZDZHJXYHY-UHFFFAOYSA-N

Formula: C14H17F4NO

SMILES: CCCCCN(C)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 291.28

Physical Properties

Property code	Value	Unit	Source
gf	-634.39	kJ/mol	Joback Method
hf	-956.94	kJ/mol	Joback Method
hfus	34.80	kJ/mol	Joback Method
hvap	54.58	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.107		Crippen Method
mcvol	202.990	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
tb	616.52	K	Joback Method
tc	795.82	K	Joback Method
tf	386.18	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.73	J/mol×K	616.52	Joback Method
cpg	554.32	J/mol×K	646.40	Joback Method
cpg	568.06	J/mol×K	676.29	Joback Method
cpg	581.00	J/mol×K	706.17	Joback Method
cpg	593.17	J/mol×K	736.05	Joback Method
cpg	604.62	J/mol×K	765.94	Joback Method
cpg	615.38	J/mol×K	795.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415524&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