2-Fluoro-6-trifluoromethylbenzamide, N-pentyl-

Inchi: InChI=1S/C13H15F4NO/c1-2-3-4-8-18-12(19)11-9(13(15,16)17)6-5-7-10(11)14/h5-7H,2-

InchiKey: QYVDFWOTLLWQCX-UHFFFAOYSA-N

Formula: C13H15F4NO

SMILES: CCCCCNC(=O)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 277.26

Physical Properties

Property code	Value	Unit	Source
gf	-664.20	kJ/mol	Joback Method
hf	-950.36	kJ/mol	Joback Method
hfus	34.29	kJ/mol	Joback Method
hvap	56.75	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.764		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
tb	631.37	K	Joback Method
tc	815.64	K	Joback Method
tf	395.10	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.81	J/mol×K	631.37	Joback Method
cpg	518.17	J/mol×K	662.08	Joback Method
cpg	530.75	J/mol×K	692.79	Joback Method
cpg	542.57	J/mol×K	723.50	Joback Method
cpg	553.66	J/mol×K	754.22	Joback Method
cpg	564.08	J/mol×K	784.93	Joback Method
cpg	573.85	J/mol×K	815.64	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=U358111&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume