2,4,5-Trifluoro-3-methoxybenzamide, N-pentyl-

Inchi: InChI=1S/C13H16F3NO2/c1-3-4-5-6-17-13(18)8-7-9(14)11(16)12(19-2)10(8)15/h7H,3-6H
InchiKey: GHACOAOPPXZYQQ-UHFFFAOYSA-N
Formula: C13H16F3NO2
SMILES: CCCCCNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 275.27

Physical Properties

Property code	Value	Unit	Source
gf	-596.49	kJ/mol	Joback Method
hf	-900.66	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	62.60	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.032		Crippen Method
mcvol	193.000	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	667.71	K	Joback Method
tc	851.78	K	Joback Method
tf	439.36	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.46	J/mol×K	667.71	Joback Method
cpg	531.41	J/mol×K	698.39	Joback Method
cpg	543.70	J/mol×K	729.07	Joback Method
cpg	555.35	J/mol×K	759.74	Joback Method
cpg	566.37	J/mol×K	790.42	Joback Method
cpg	576.75	J/mol×K	821.10	Joback Method
cpg	586.50	J/mol×K	851.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358063&Units=SI

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