Benzamide, 2,4,5-trifluoro-3-methoxy-N-hexyl-

Inchi: InChI=1S/C14H18F3NO2/c1-3-4-5-6-7-18-14(19)9-8-10(15)12(17)13(20-2)11(9)16/h8H,3
InchiKey: PSJYIWMRCSINIU-UHFFFAOYSA-N
Formula: C14H18F3NO2
SMILES: CCCCCCNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 289.29

Physical Properties

Property code	Value	Unit	Source
gf	-588.07	kJ/mol	Joback Method
hf	-921.30	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	64.82	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	3.423		Crippen Method
mcvol	207.090	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	690.59	K	Joback Method
tc	873.72	K	Joback Method
tf	450.63	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.85	J/mol×K	690.59	Joback Method
cpg	584.35	J/mol×K	721.11	Joback Method
cpg	597.15	J/mol×K	751.63	Joback Method
cpg	609.27	J/mol×K	782.16	Joback Method
cpg	620.71	J/mol×K	812.68	Joback Method
cpg	631.48	J/mol×K	843.20	Joback Method
cpg	641.59	J/mol×K	873.72	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=U407642&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