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

Inchi: InChI=1S/C17H24F3NO2/c1-3-4-5-6-7-8-9-10-21-17(22)12-11-13(18)15(20)16(23-2)14(1
InchiKey: FNJZKCDREHVUHW-UHFFFAOYSA-N
Formula: C17H24F3NO2
SMILES: CCCCCCCCCNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 331.37

Physical Properties

Property code	Value	Unit	Source
gf	-562.81	kJ/mol	Joback Method
hf	-983.22	kJ/mol	Joback Method
hfus	49.40	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	4.593		Crippen Method
mcvol	249.360	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	759.23	K	Joback Method
tc	942.43	K	Joback Method
tf	484.44	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.44	J/mol×K	759.23	Joback Method
cpg	750.34	J/mol×K	789.76	Joback Method
cpg	764.41	J/mol×K	820.30	Joback Method
cpg	777.68	J/mol×K	850.83	Joback Method
cpg	790.15	J/mol×K	881.36	Joback Method
cpg	801.84	J/mol×K	911.89	Joback Method
cpg	812.76	J/mol×K	942.43	Joback Method

Sources

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=U407646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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