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

Inchi: InChI=1S/C22H34F3NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-26-22(27)17-16-18(23)20(

InchiKey: RWDVBKXKGWQQKE-UHFFFAOYSA-N

Formula: C22H34F3NO2

SMILES: CCCCCCCCCCCCCCNC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 401.51

Physical Properties

Property code	Value	Unit	Source
gf	-520.71	kJ/mol	Joback Method
hf	-1086.42	kJ/mol	Joback Method
hfus	62.35	kJ/mol	Joback Method
hvap	82.63	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	6.543		Crippen Method
mcvol	319.810	ml/mol	McGowan Method
pc	1017.48	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	873.63	K	Joback Method
tc	1069.74	K	Joback Method
tf	540.79	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.57	J/mol×K	873.63	Joback Method
cpg	1046.59	J/mol×K	906.31	Joback Method
cpg	1062.48	J/mol×K	939.00	Joback Method
cpg	1077.29	J/mol×K	971.68	Joback Method
cpg	1091.04	J/mol×K	1004.37	Joback Method
cpg	1103.76	J/mol×K	1037.05	Joback Method
cpg	1115.47	J/mol×K	1069.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407650&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

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