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

Inchi: InChI=1S/C24H38F3NO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-28-24(29)19-18-20(

InchiKey: XVTDJYOFSBKGNY-UHFFFAOYSA-N

Formula: C24H38F3NO2

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

Mol. weight [g/mol]: 429.56

Physical Properties

Property code	Value	Unit	Source
gf	-503.87	kJ/mol	Joback Method
hf	-1127.70	kJ/mol	Joback Method
hfus	67.53	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	7.324		Crippen Method
mcvol	347.990	ml/mol	McGowan Method
pc	903.43	kPa	Joback Method
rinpol	2957.00		NIST Webbook
rinpol	2957.00		NIST Webbook
tb	919.39	K	Joback Method
tc	1126.56	K	Joback Method
tf	563.33	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.47	J/mol×K	919.39	Joback Method
cpg	1170.46	J/mol×K	953.92	Joback Method
cpg	1187.14	J/mol×K	988.45	Joback Method
cpg	1202.57	J/mol×K	1022.97	Joback Method
cpg	1216.79	J/mol×K	1057.50	Joback Method
cpg	1229.82	J/mol×K	1092.03	Joback Method
cpg	1241.72	J/mol×K	1126.56	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=U407651&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