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

Inchi: InChI=1S/C20H30F3NO2/c1-4-6-8-10-12-24(13-11-9-7-5-2)20(25)15-14-16(21)18(23)19(

InchiKey: RTLJTRVADIWHON-UHFFFAOYSA-N

Formula: C20H30F3NO2

SMILES: CCCCCCN(CCCCCC)C(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 373.45

Physical Properties

Property code	Value	Unit	Source
gf	-516.16	kJ/mol	Joback Method
hf	-1031.08	kJ/mol	Joback Method
hfus	55.09	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.715		Crippen Method
mcvol	291.630	ml/mol	McGowan Method
pc	1142.89	kPa	Joback Method
rinpol	2311.00		NIST Webbook
tb	790.14	K	Joback Method
tc	972.62	K	Joback Method
tf	498.06	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.24	J/mol×K	790.14	Joback Method
cpg	906.94	J/mol×K	820.55	Joback Method
cpg	922.71	J/mol×K	850.97	Joback Method
cpg	937.57	J/mol×K	881.38	Joback Method
cpg	951.53	J/mol×K	911.79	Joback Method
cpg	964.63	J/mol×K	942.21	Joback Method
cpg	976.89	J/mol×K	972.62	Joback Method

Sources

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=U358067&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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