2,4,5-Trifluoro-3-methoxybenzamide, N,N-di(2-ethylhexyl)-

Inchi: InChI=1S/C24H38F3NO2/c1-6-10-12-17(8-3)15-28(16-18(9-4)13-11-7-2)24(29)19-14-20(
InchiKey: SRJHWNRIHZOGQR-UHFFFAOYSA-N
Formula: C24H38F3NO2
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 429.56

Physical Properties

Property code	Value	Unit	Source
gf	-487.36	kJ/mol	Joback Method
hf	-1124.20	kJ/mol	Joback Method
hfus	58.40	kJ/mol	Joback Method
hvap	81.91	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.987		Crippen Method
mcvol	347.990	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	2461.00		NIST Webbook
tb	880.78	K	Joback Method
tc	1078.36	K	Joback Method
tf	513.14	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.47	J/mol×K	880.78	Joback Method
cpg	1151.95	J/mol×K	913.71	Joback Method
cpg	1169.20	J/mol×K	946.64	Joback Method
cpg	1185.27	J/mol×K	979.57	Joback Method
cpg	1200.20	J/mol×K	1012.50	Joback Method
cpg	1214.02	J/mol×K	1045.43	Joback Method
cpg	1226.79	J/mol×K	1078.36	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=U358069&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