2,4,5-Trifluoro-3-methoxybenzoic acid, 2-ethylhexyl ester

Inchi: InChI=1S/C16H21F3O3/c1-4-6-7-10(5-2)9-22-16(20)11-8-12(17)14(19)15(21-3)13(11)18

InchiKey: MEWBYBUKMFLKMO-UHFFFAOYSA-N

Formula: C16H21F3O3

SMILES: CCCCC(CC)COC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 318.33

Physical Properties

Property code	Value	Unit	Source
gf	-768.06	kJ/mol	Joback Method
hf	-1153.55	kJ/mol	Joback Method
hfus	39.37	kJ/mol	Joback Method
hvap	64.86	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.486		Crippen Method
mcvol	231.160	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	708.16	K	Joback Method
tc	889.80	K	Joback Method
tf	427.74	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.90	J/mol×K	708.16	Joback Method
cpg	665.69	J/mol×K	738.43	Joback Method
cpg	679.72	J/mol×K	768.71	Joback Method
cpg	692.99	J/mol×K	798.98	Joback Method
cpg	705.51	J/mol×K	829.25	Joback Method
cpg	717.26	J/mol×K	859.52	Joback Method
cpg	728.25	J/mol×K	889.80	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=U357612&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