3-Methoxy-2,4,5-trifluorobenzoic acid, decyl ester

Inchi: InChI=1S/C18H25F3O3/c1-3-4-5-6-7-8-9-10-11-24-18(22)13-12-14(19)16(21)17(23-2)15

InchiKey: UXZLLTILUQVRNI-UHFFFAOYSA-N

Formula: C18H25F3O3

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

Mol. weight [g/mol]: 346.38

Physical Properties

Property code	Value	Unit	Source
gf	-748.78	kJ/mol	Joback Method
hf	-1189.55	kJ/mol	Joback Method
hfus	48.08	kJ/mol	Joback Method
hvap	69.70	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.410		Crippen Method
mcvol	259.340	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	754.36	K	Joback Method
tc	934.90	K	Joback Method
tf	465.28	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.23	J/mol×K	754.36	Joback Method
cpg	777.73	J/mol×K	784.45	Joback Method
cpg	792.39	J/mol×K	814.54	Joback Method
cpg	806.22	J/mol×K	844.63	Joback Method
cpg	819.22	J/mol×K	874.72	Joback Method
cpg	831.39	J/mol×K	904.81	Joback Method
cpg	842.74	J/mol×K	934.90	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=U338767&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

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