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

Inchi: InChI=1S/C28H45F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-34-28(3

InchiKey: NQUBKJPFVOGFSM-UHFFFAOYSA-N

Formula: C28H45F3O3

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

Mol. weight [g/mol]: 486.65

Physical Properties

Property code	Value	Unit	Source
gf	-664.58	kJ/mol	Joback Method
hf	-1395.95	kJ/mol	Joback Method
hfus	73.98	kJ/mol	Joback Method
hvap	91.96	kJ/mol	Joback Method
log10ws	-10.78		Crippen Method
logp	9.311		Crippen Method
mcvol	400.240	ml/mol	McGowan Method
pc	714.54	kPa	Joback Method
rinpol	3241.00		NIST Webbook
tb	983.16	K	Joback Method
tc	1215.56	K	Joback Method
tf	577.98	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1371.41	J/mol×K	983.16	Joback Method
cpg	1391.59	J/mol×K	1021.89	Joback Method
cpg	1409.91	J/mol×K	1060.63	Joback Method
cpg	1426.40	J/mol×K	1099.36	Joback Method
cpg	1441.13	J/mol×K	1138.09	Joback Method
cpg	1454.14	J/mol×K	1176.82	Joback Method
cpg	1465.48	J/mol×K	1215.56	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=U338777&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