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

Inchi: InChI=1S/C15H19F3O3/c1-3-4-5-6-7-8-21-15(19)10-9-11(16)13(18)14(20-2)12(10)17/h9
InchiKey: ZPOZCTMUMLAWOD-UHFFFAOYSA-N
Formula: C15H19F3O3
SMILES: CCCCCCCOC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 304.30

Physical Properties

Property code	Value	Unit	Source
gf	-774.04	kJ/mol	Joback Method
hf	-1127.63	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	63.02	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.240		Crippen Method
mcvol	217.070	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
tb	685.72	K	Joback Method
tc	865.40	K	Joback Method
tf	431.47	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.23	J/mol×K	685.72	Joback Method
cpg	610.32	J/mol×K	715.67	Joback Method
cpg	623.73	J/mol×K	745.61	Joback Method
cpg	636.44	J/mol×K	775.56	Joback Method
cpg	648.47	J/mol×K	805.50	Joback Method
cpg	659.81	J/mol×K	835.45	Joback Method
cpg	670.45	J/mol×K	865.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338764&Units=SI
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

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