

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

Inchi:	InChI=1S/C14H17F3O3/c1-3-4-5-6-7-20-14(18)9-8-10(15)12(17)13(19-2)11(9)16/h8H,3-
InchiKey:	NAJHYJASSWBYIF-UHFFFAOYSA-N
Formula:	C14H17F3O3
SMILES:	CCCCCOC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]:	290.28

Physical Properties

Property code	Value	Unit	Source
gf	-782.46	kJ/mol	Joback Method
hf	-1106.99	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.850		Crippen Method
mcvol	202.980	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
tb	662.84	K	Joback Method
tc	843.19	K	Joback Method
tf	420.20	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.38	J/molxK	662.84	Joback Method
cpg	556.92	J/molxK	692.90	Joback Method
cpg	569.81	J/molxK	722.96	Joback Method
cpg	582.07	J/molxK	753.01	Joback Method
cpg	593.69	J/molxK	783.07	Joback Method
cpg	604.65	J/molxK	813.13	Joback Method
cpg	614.97	J/molxK	843.19	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=U338763&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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