3-Methoxy-2,4,5-trifluorobenzoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C16H20ClF3O3/c1-22-15-13(19)11(10-12(18)14(15)20)16(21)23-9-7-5-3-2-4-6

InchiKey: WARDNNXIUFMWSE-UHFFFAOYSA-N

Formula: C16H20ClF3O3

SMILES: COc1c(F)c(F)cc(C(=O)OCCCCCCCCCl)c1F

Mol. weight [g/mol]: 352.78

Physical Properties

Property code	Value	Unit	Source
gf	-777.55	kJ/mol	Joback Method
hf	-1164.01	kJ/mol	Joback Method
hfus	47.09	kJ/mol	Joback Method
hvap	69.63	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.849		Crippen Method
mcvol	243.400	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2259.00		NIST Webbook
rinpol	2259.00		NIST Webbook
tb	746.03	K	Joback Method
tc	930.33	K	Joback Method
tf	472.66	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.87	J/mol×K	746.03	Joback Method
cpg	692.64	J/mol×K	776.75	Joback Method
cpg	705.63	J/mol×K	807.46	Joback Method
cpg	717.86	J/mol×K	838.18	Joback Method
cpg	729.31	J/mol×K	868.90	Joback Method
cpg	740.00	J/mol×K	899.61	Joback Method
cpg	749.92	J/mol×K	930.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360574&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

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