2-Fluoro-3-trifluoromethylbenzoic acid, octyl ester

Inchi: InChI=1S/C16H20F4O2/c1-2-3-4-5-6-7-11-22-15(21)12-9-8-10-13(14(12)17)16(18,19)20

InchiKey: BBTMRZAYPYFDDQ-UHFFFAOYSA-N

Formula: C16H20F4O2

SMILES: CCCCCCCCOC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 320.32

Physical Properties

Property code	Value	Unit	Source
gf	-833.33	kJ/mol	Joback Method
hf	-1197.97	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	59.40	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.362		Crippen Method
mcvol	227.060	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	672.26	K	Joback Method
tc	850.60	K	Joback Method
tf	398.48	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.67	J/mol×K	672.26	Joback Method
cpg	648.54	J/mol×K	701.98	Joback Method
cpg	662.59	J/mol×K	731.71	Joback Method
cpg	675.86	J/mol×K	761.43	Joback Method
cpg	688.38	J/mol×K	791.15	Joback Method
cpg	700.16	J/mol×K	820.88	Joback Method
cpg	711.25	J/mol×K	850.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338723&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

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