3-Fluoro-4-trifluoromethylbenzoic acid, 2-ethylhexyl ester

Inchi: InChI=1S/C16H20F4O2/c1-3-5-6-11(4-2)10-22-15(21)12-7-8-13(14(17)9-12)16(18,19)20
InchiKey: QTFOYNIOELTJSW-UHFFFAOYSA-N
Formula: C16H20F4O2
SMILES: CCCCC(CC)COC(=O)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 320.32

Physical Properties

Property code	Value	Unit	Source
gf	-835.77	kJ/mol	Joback Method
hf	-1203.25	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	59.01	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.218		Crippen Method
mcvol	227.060	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1659.00		NIST Webbook
tb	671.82	K	Joback Method
tc	852.66	K	Joback Method
tf	383.48	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.14	J/mol×K	671.82	Joback Method
cpg	649.25	J/mol×K	701.96	Joback Method
cpg	663.52	J/mol×K	732.10	Joback Method
cpg	676.97	J/mol×K	762.24	Joback Method
cpg	689.63	J/mol×K	792.38	Joback Method
cpg	701.54	J/mol×K	822.52	Joback Method
cpg	712.72	J/mol×K	852.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357938&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

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