2-Fluoro-3-trifluoromethylbenzoic acid, nonadecyl ester

Inchi: InChI=1S/C27H42F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-33-26(32)23

InchiKey: VRCOUWKWKOLVRT-UHFFFAOYSA-N

Formula: C27H42F4O2

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

Mol. weight [g/mol]: 474.61

Physical Properties

Property code	Value	Unit	Source
gf	-740.71	kJ/mol	Joback Method
hf	-1425.01	kJ/mol	Joback Method
hfus	66.64	kJ/mol	Joback Method
hvap	83.89	kJ/mol	Joback Method
log10ws	-10.68		Crippen Method
logp	9.653		Crippen Method
mcvol	382.050	ml/mol	McGowan Method
pc	761.42	kPa	Joback Method
rinpol	2874.00		NIST Webbook
rinpol	2874.00		NIST Webbook
tb	923.94	K	Joback Method
tc	1134.00	K	Joback Method
tf	522.45	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.74	J/mol×K	923.94	Joback Method
cpg	1303.48	J/mol×K	958.95	Joback Method
cpg	1321.90	J/mol×K	993.96	Joback Method
cpg	1339.07	J/mol×K	1028.97	Joback Method
cpg	1355.09	J/mol×K	1063.98	Joback Method
cpg	1370.02	J/mol×K	1098.99	Joback Method
cpg	1383.96	J/mol×K	1134.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338734&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