5-Fluoro-3-trifluoromethylbenzoic acid, octadecyl ester

Inchi: InChI=1S/C26H40F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-32-25(31)22-19

InchiKey: BISSECQBHZYFHV-UHFFFAOYSA-N

Formula: C26H40F4O2

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 460.59

Physical Properties

Property code	Value	Unit	Source
gf	-749.13	kJ/mol	Joback Method
hf	-1404.37	kJ/mol	Joback Method
hfus	64.05	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-10.27		Crippen Method
logp	9.263		Crippen Method
mcvol	367.960	ml/mol	McGowan Method
pc	803.42	kPa	Joback Method
rinpol	2632.00		NIST Webbook
rinpol	2632.00		NIST Webbook
tb	901.06	K	Joback Method
tc	1104.09	K	Joback Method
tf	511.18	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.85	J/mol×K	901.06	Joback Method
cpg	1239.98	J/mol×K	934.90	Joback Method
cpg	1257.87	J/mol×K	968.74	Joback Method
cpg	1274.59	J/mol×K	1002.57	Joback Method
cpg	1290.21	J/mol×K	1036.41	Joback Method
cpg	1304.80	J/mol×K	1070.25	Joback Method
cpg	1318.43	J/mol×K	1104.09	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=U338910&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume