2-Fluoro-5-trifluoromethylbenzoic acid, eicosyl ester

Inchi: InChI=1S/C28H44F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-34-27(33

InchiKey: YDDXEPMOLAKKSN-UHFFFAOYSA-N

Formula: C28H44F4O2

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]: 488.64

Physical Properties

Property code	Value	Unit	Source
gf	-732.29	kJ/mol	Joback Method
hf	-1445.65	kJ/mol	Joback Method
hfus	69.23	kJ/mol	Joback Method
hvap	86.11	kJ/mol	Joback Method
log10ws	-11.10		Crippen Method
logp	10.043		Crippen Method
mcvol	396.140	ml/mol	McGowan Method
pc	722.63	kPa	Joback Method
rinpol	2900.00		NIST Webbook
rinpol	2900.00		NIST Webbook
tb	946.82	K	Joback Method
tc	1165.03	K	Joback Method
tf	533.72	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.17	J/mol×K	946.82	Joback Method
cpg	1367.59	J/mol×K	983.19	Joback Method
cpg	1386.59	J/mol×K	1019.56	Joback Method
cpg	1404.26	J/mol×K	1055.93	Joback Method
cpg	1420.71	J/mol×K	1092.30	Joback Method
cpg	1436.02	J/mol×K	1128.66	Joback Method
cpg	1450.30	J/mol×K	1165.03	Joback Method

Sources

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=U338974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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