2-Fluoro-5-trifluoromethylbenzoic acid, heptadecyl ester

Inchi: InChI=1S/C25H38F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-31-24(30)22-20-21

InchiKey: UQSLALKTOKSEIM-UHFFFAOYSA-N

Formula: C25H38F4O2

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

Mol. weight [g/mol]: 446.56

Physical Properties

Property code	Value	Unit	Source
gf	-757.55	kJ/mol	Joback Method
hf	-1383.73	kJ/mol	Joback Method
hfus	61.46	kJ/mol	Joback Method
hvap	79.44	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	8.873		Crippen Method
mcvol	353.870	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	878.18	K	Joback Method
tc	1075.21	K	Joback Method
tf	499.91	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.56	J/mol×K	878.18	Joback Method
cpg	1177.13	J/mol×K	911.02	Joback Method
cpg	1194.54	J/mol×K	943.86	Joback Method
cpg	1210.84	J/mol×K	976.70	Joback Method
cpg	1226.09	J/mol×K	1009.53	Joback Method
cpg	1240.36	J/mol×K	1042.37	Joback Method
cpg	1253.72	J/mol×K	1075.21	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=U338971&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