2,5-Di(trifluoromethyl)benzoic acid, octadecyl ester

Inchi: InChI=1S/C27H40F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-35-25(34)23-21
InchiKey: CFGLSOQDGACDGX-UHFFFAOYSA-N
Formula: C27H40F6O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 510.60

Physical Properties

Property code	Value	Unit	Source
gf	-1127.49	kJ/mol	Joback Method
hf	-1825.98	kJ/mol	Joback Method
hfus	65.39	kJ/mol	Joback Method
hvap	80.96	kJ/mol	Joback Method
log10ws	-11.04		Crippen Method
logp	10.143		Crippen Method
mcvol	385.590	ml/mol	McGowan Method
pc	732.44	kPa	Joback Method
rinpol	2611.00		NIST Webbook
tb	919.25	K	Joback Method
tc	1129.63	K	Joback Method
tf	526.05	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.69	J/mol×K	919.25	Joback Method
cpg	1317.12	J/mol×K	954.31	Joback Method
cpg	1335.29	J/mol×K	989.38	Joback Method
cpg	1352.30	J/mol×K	1024.44	Joback Method
cpg	1368.26	J/mol×K	1059.51	Joback Method
cpg	1383.28	J/mol×K	1094.57	Joback Method
cpg	1397.46	J/mol×K	1129.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338951&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

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