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

Inchi: InChI=1S/C29H44F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-37-27(36
InchiKey: SYQGQADEAWYMHS-UHFFFAOYSA-N
Formula: C29H44F6O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 538.65

Physical Properties

Property code	Value	Unit	Source
gf	-1110.65	kJ/mol	Joback Method
hf	-1867.26	kJ/mol	Joback Method
hfus	70.57	kJ/mol	Joback Method
hvap	85.41	kJ/mol	Joback Method
log10ws	-11.87		Crippen Method
logp	10.923		Crippen Method
mcvol	413.770	ml/mol	McGowan Method
pc	661.87	kPa	Joback Method
rinpol	2796.00		NIST Webbook
rinpol	2796.00		NIST Webbook
tb	965.01	K	Joback Method
tc	1194.09	K	Joback Method
tf	548.59	K	Joback Method
vc	1.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1424.39	J/mol×K	965.01	Joback Method
cpg	1445.44	J/mol×K	1003.19	Joback Method
cpg	1465.06	J/mol×K	1041.37	Joback Method
cpg	1483.40	J/mol×K	1079.55	Joback Method
cpg	1500.59	J/mol×K	1117.73	Joback Method
cpg	1516.78	J/mol×K	1155.91	Joback Method
cpg	1532.10	J/mol×K	1194.09	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=U338953&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