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

Inchi: InChI=1S/C23H32F6O2/c1-3-4-5-6-7-8-9-10-11-12-13-17(2)31-21(30)19-16-18(22(24,25
InchiKey: SWCQAJLFQDKBPF-UHFFFAOYSA-N
Formula: C23H32F6O2
SMILES: CCCCCCCCCCCCC(C)OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 454.49

Physical Properties

Property code	Value	Unit	Source
gf	-1163.61	kJ/mol	Joback Method
hf	-1748.70	kJ/mol	Joback Method
hfus	51.51	kJ/mol	Joback Method
hvap	71.67	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	8.581		Crippen Method
mcvol	329.230	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	827.29	K	Joback Method
tc	1013.79	K	Joback Method
tf	465.97	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.01	J/mol×K	827.29	Joback Method
cpg	1069.08	J/mol×K	858.37	Joback Method
cpg	1085.12	J/mol×K	889.46	Joback Method
cpg	1100.19	J/mol×K	920.54	Joback Method
cpg	1114.35	J/mol×K	951.62	Joback Method
cpg	1127.66	J/mol×K	982.70	Joback Method
cpg	1140.20	J/mol×K	1013.79	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=U338706&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