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

Inchi: InChI=1S/C25H36F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-33-23(32)21-19-20(24
InchiKey: UHCXVSPHICTBQZ-UHFFFAOYSA-N
Formula: C25H36F6O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 482.54

Physical Properties

Property code	Value	Unit	Source
gf	-1144.33	kJ/mol	Joback Method
hf	-1784.70	kJ/mol	Joback Method
hfus	60.21	kJ/mol	Joback Method
hvap	76.51	kJ/mol	Joback Method
log10ws	-10.20		Crippen Method
logp	9.362		Crippen Method
mcvol	357.410	ml/mol	McGowan Method
pc	814.93	kPa	Joback Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
tb	873.49	K	Joback Method
tc	1069.79	K	Joback Method
tf	503.51	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1173.29	J/mol×K	873.49	Joback Method
cpg	1191.40	J/mol×K	906.21	Joback Method
cpg	1208.39	J/mol×K	938.92	Joback Method
cpg	1224.34	J/mol×K	971.64	Joback Method
cpg	1239.32	J/mol×K	1004.36	Joback Method
cpg	1253.41	J/mol×K	1037.08	Joback Method
cpg	1266.70	J/mol×K	1069.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338949&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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