2,5-Di(trifluoromethyl)benzoic acid, 4-hexadecyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-1146.77	kJ/mol	Joback Method
hf	-1789.98	kJ/mol	Joback Method
hfus	56.68	kJ/mol	Joback Method
hvap	76.12	kJ/mol	Joback Method
log10ws	-10.31		Crippen Method
logp	9.361		Crippen Method
mcvol	357.410	ml/mol	McGowan Method
pc	818.66	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	873.05	K	Joback Method
tc	1068.99	K	Joback Method
tf	488.51	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1173.75	J/mol×K	873.05	Joback Method
cpg	1191.82	J/mol×K	905.71	Joback Method
cpg	1208.75	J/mol×K	938.36	Joback Method
cpg	1224.64	J/mol×K	971.02	Joback Method
cpg	1239.55	J/mol×K	1003.68	Joback Method
cpg	1253.56	J/mol×K	1036.33	Joback Method
cpg	1266.76	J/mol×K	1068.99	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=U338715&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