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

Inchi: InChI=1S/C28H42F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-36-26(35)24
InchiKey: IKPCTGOLZBVXMQ-UHFFFAOYSA-N
Formula: C28H42F6O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 524.62

Physical Properties

Property code	Value	Unit	Source
gf	-1119.07	kJ/mol	Joback Method
hf	-1846.62	kJ/mol	Joback Method
hfus	67.98	kJ/mol	Joback Method
hvap	83.18	kJ/mol	Joback Method
log10ws	-11.46		Crippen Method
logp	10.533		Crippen Method
mcvol	399.680	ml/mol	McGowan Method
pc	695.81	kPa	Joback Method
rinpol	2703.00		NIST Webbook
rinpol	2703.00		NIST Webbook
tb	942.13	K	Joback Method
tc	1161.24	K	Joback Method
tf	537.32	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1360.78	J/mol×K	942.13	Joback Method
cpg	1380.97	J/mol×K	978.65	Joback Method
cpg	1399.82	J/mol×K	1015.17	Joback Method
cpg	1417.46	J/mol×K	1051.68	Joback Method
cpg	1434.01	J/mol×K	1088.20	Joback Method
cpg	1449.57	J/mol×K	1124.72	Joback Method
cpg	1464.28	J/mol×K	1161.24	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=U338952&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