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

Inchi: InChI=1S/C21H28F6O2/c1-2-3-4-5-6-7-8-9-10-11-14-29-19(28)17-15-16(20(22,23)24)12
InchiKey: AYZAWZDTNFCYQN-UHFFFAOYSA-N
Formula: C21H28F6O2
SMILES: CCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 426.44

Physical Properties

Property code	Value	Unit	Source
gf	-1178.01	kJ/mol	Joback Method
hf	-1702.14	kJ/mol	Joback Method
hfus	49.85	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.802		Crippen Method
mcvol	301.050	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	781.97	K	Joback Method
tc	961.34	K	Joback Method
tf	458.43	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.77	J/mol×K	781.97	Joback Method
cpg	948.93	J/mol×K	811.86	Joback Method
cpg	964.13	J/mol×K	841.76	Joback Method
cpg	978.45	J/mol×K	871.65	Joback Method
cpg	991.92	J/mol×K	901.55	Joback Method
cpg	1004.61	J/mol×K	931.44	Joback Method
cpg	1016.56	J/mol×K	961.34	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=U338945&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