2,5-Di(trifluoromethyl)benzoic acid, 3-dodecyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-1180.45	kJ/mol	Joback Method
hf	-1707.42	kJ/mol	Joback Method
hfus	46.32	kJ/mol	Joback Method
hvap	67.21	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	7.800		Crippen Method
mcvol	301.050	ml/mol	McGowan Method
pc	1033.24	kPa	Joback Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
tb	781.53	K	Joback Method
tc	961.86	K	Joback Method
tf	443.43	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.28	J/mol×K	781.53	Joback Method
cpg	949.53	J/mol×K	811.59	Joback Method
cpg	964.81	J/mol×K	841.64	Joback Method
cpg	979.19	J/mol×K	871.70	Joback Method
cpg	992.70	J/mol×K	901.75	Joback Method
cpg	1005.41	J/mol×K	931.81	Joback Method
cpg	1017.37	J/mol×K	961.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338696&Units=SI

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