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

Inchi: InChI=1S/C22H30F6O2/c1-3-5-6-7-8-9-10-12-17(11-4-2)30-20(29)18-15-16(21(23,24)25
InchiKey: LWVBGODBXGEKMD-UHFFFAOYSA-N
Formula: C22H30F6O2
SMILES: CCCCCCCCCC(CCC)OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 440.46

Physical Properties

Property code	Value	Unit	Source
gf	-1172.03	kJ/mol	Joback Method
hf	-1728.06	kJ/mol	Joback Method
hfus	48.91	kJ/mol	Joback Method
hvap	69.44	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	8.190		Crippen Method
mcvol	315.140	ml/mol	McGowan Method
pc	972.30	kPa	Joback Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	804.41	K	Joback Method
tc	987.45	K	Joback Method
tf	454.70	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.24	J/mol×K	804.41	Joback Method
cpg	1008.88	J/mol×K	834.92	Joback Method
cpg	1024.53	J/mol×K	865.42	Joback Method
cpg	1039.24	J/mol×K	895.93	Joback Method
cpg	1053.07	J/mol×K	926.44	Joback Method
cpg	1066.07	J/mol×K	956.94	Joback Method
cpg	1078.31	J/mol×K	987.45	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=U338702&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