Terephthalic acid, decyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C24H27F3O4/c1-2-3-4-5-6-7-8-9-16-30-23(28)17-10-12-18(13-11-17)24(29)31
InchiKey: SMWSVVQOROZWFM-UHFFFAOYSA-N
Formula: C24H27F3O4
SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)Oc2ccc(F)c(F)c2F)cc1
Mol. weight [g/mol]: 436.46

Physical Properties

Property code	Value	Unit	Source
gf	-714.77	kJ/mol	Joback Method
hf	-1189.44	kJ/mol	Joback Method
hfus	59.26	kJ/mol	Joback Method
hvap	92.08	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	6.621		Crippen Method
mcvol	321.690	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	972.19	K	Joback Method
tc	1190.84	K	Joback Method
tf	609.25	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.30	J/mol×K	972.19	Joback Method
cpg	1047.57	J/mol×K	1008.63	Joback Method
cpg	1059.46	J/mol×K	1045.07	Joback Method
cpg	1070.01	J/mol×K	1081.52	Joback Method
cpg	1079.26	J/mol×K	1117.96	Joback Method
cpg	1087.22	J/mol×K	1154.40	Joback Method
cpg	1093.95	J/mol×K	1190.84	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=U415806&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