Terephthalic acid, octyl 3,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C23H25F3O4/c1-2-3-4-5-6-7-12-29-22(27)17-8-10-18(11-9-17)23(28)30-15-16
InchiKey: BMVSTLWDAADMAA-UHFFFAOYSA-N
Formula: C23H25F3O4
SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OCc2cc(F)c(F)c(F)c2)cc1
Mol. weight [g/mol]: 422.44

Physical Properties

Property code	Value	Unit	Source
gf	-723.19	kJ/mol	Joback Method
hf	-1168.80	kJ/mol	Joback Method
hfus	56.67	kJ/mol	Joback Method
hvap	89.85	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	5.978		Crippen Method
mcvol	307.600	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpol	3276.00		NIST Webbook
rinpol	3276.00		NIST Webbook
tb	949.31	K	Joback Method
tc	1164.42	K	Joback Method
tf	597.98	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.81	J/mol×K	949.31	Joback Method
cpg	987.92	J/mol×K	985.16	Joback Method
cpg	999.72	J/mol×K	1021.01	Joback Method
cpg	1010.24	J/mol×K	1056.87	Joback Method
cpg	1019.52	J/mol×K	1092.72	Joback Method
cpg	1027.58	J/mol×K	1128.57	Joback Method
cpg	1034.46	J/mol×K	1164.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382887&Units=SI
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

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