Terephthalic acid, octyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C24H25F5O4/c1-3-4-5-6-7-8-13-32-23(30)15-9-11-16(12-10-15)24(31)33-14(2

InchiKey: GEFJOOGVFAZFQY-UHFFFAOYSA-N

Formula: C24H25F5O4

SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OC(C)c2c(F)c(F)c(F)c(F)c2F)cc1

Mol. weight [g/mol]: 472.44

Physical Properties

Property code	Value	Unit	Source
gf	-1126.09	kJ/mol	Joback Method
hf	-1609.88	kJ/mol	Joback Method
hfus	61.12	kJ/mol	Joback Method
hvap	91.38	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	6.817		Crippen Method
mcvol	325.230	ml/mol	McGowan Method
pc	1057.57	kPa	Joback Method
rinpol	2854.00		NIST Webbook
rinpol	2854.00		NIST Webbook
tb	980.25	K	Joback Method
tc	1200.17	K	Joback Method
tf	620.47	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.15	J/mol×K	980.25	Joback Method
cpg	1058.80	J/mol×K	1016.90	Joback Method
cpg	1070.00	J/mol×K	1053.56	Joback Method
cpg	1079.79	J/mol×K	1090.21	Joback Method
cpg	1088.18	J/mol×K	1126.86	Joback Method
cpg	1095.20	J/mol×K	1163.51	Joback Method
cpg	1100.86	J/mol×K	1200.17	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=U416060&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