Terephthalic acid, nonyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C25H27F5O4/c1-3-4-5-6-7-8-9-14-33-24(31)16-10-12-17(13-11-16)25(32)34-1

InchiKey: ZOUJPPXNBAMFKD-UHFFFAOYSA-N

Formula: C25H27F5O4

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

Mol. weight [g/mol]: 486.47

Physical Properties

Property code	Value	Unit	Source
gf	-1117.67	kJ/mol	Joback Method
hf	-1630.52	kJ/mol	Joback Method
hfus	63.70	kJ/mol	Joback Method
hvap	93.61	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	7.207		Crippen Method
mcvol	339.320	ml/mol	McGowan Method
pc	994.51	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	1003.13	K	Joback Method
tc	1229.10	K	Joback Method
tf	631.74	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1105.88	J/mol×K	1003.13	Joback Method
cpg	1118.72	J/mol×K	1040.79	Joback Method
cpg	1130.00	J/mol×K	1078.45	Joback Method
cpg	1139.76	J/mol×K	1116.11	Joback Method
cpg	1148.02	J/mol×K	1153.78	Joback Method
cpg	1154.81	J/mol×K	1191.44	Joback Method
cpg	1160.16	J/mol×K	1229.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416061&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

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