Terephthalic acid, di(1-(pentafluorophenyl)ethyl) ester

Inchi: InChI=1S/C24H12F10O4/c1-7(11-13(25)17(29)21(33)18(30)14(11)26)37-23(35)9-3-5-10

InchiKey: VTXNWHSDQPMDLB-UHFFFAOYSA-N

Formula: C24H12F10O4

SMILES: CC(OC(=O)c1ccc(C(=O)OC(C)c2c(F)c(F)c(F)c(F)c2F)cc1)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 554.33

Physical Properties

Property code	Value	Unit	Source
gf	-2038.32	kJ/mol	Joback Method
hf	-2416.53	kJ/mol	Joback Method
hfus	65.09	kJ/mol	Joback Method
hvap	92.49	kJ/mol	Joback Method
log10ws	-10.26		Crippen Method
logp	6.914		Crippen Method
mcvol	310.320	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	2554.00		NIST Webbook
rinpol	2554.00		NIST Webbook
tb	1027.74	K	Joback Method
tc	1259.83	K	Joback Method
tf	697.44	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	961.97	J/mol×K	1027.74	Joback Method
cpg	969.89	J/mol×K	1066.42	Joback Method
cpg	976.20	J/mol×K	1105.10	Joback Method
cpg	980.92	J/mol×K	1143.79	Joback Method
cpg	984.03	J/mol×K	1182.47	Joback Method
cpg	985.55	J/mol×K	1221.15	Joback Method
cpg	985.48	J/mol×K	1259.83	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=U416062&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