Pimelic acid, 4-methyl-2-pentyl pentafluorobenzyl ester

Inchi: InChI=1S/C20H25F5O4/c1-11(2)9-12(3)29-15(27)8-6-4-5-7-14(26)28-10-13-16(21)18(23
InchiKey: UMJHPPZMABXYRR-UHFFFAOYSA-N
Formula: C20H25F5O4
SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 424.40

Physical Properties

Property code	Value	Unit	Source
gf	-1264.99	kJ/mol	Joback Method
hf	-1757.66	kJ/mol	Joback Method
hfus	53.58	kJ/mol	Joback Method
hvap	79.15	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.354		Crippen Method
mcvol	292.630	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2208.00		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	856.63	K	Joback Method
tc	1049.51	K	Joback Method
tf	521.45	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.66	J/mol×K	856.63	Joback Method
cpg	927.11	J/mol×K	888.78	Joback Method
cpg	940.49	J/mol×K	920.92	Joback Method
cpg	952.80	J/mol×K	953.07	Joback Method
cpg	964.06	J/mol×K	985.22	Joback Method
cpg	974.27	J/mol×K	1017.36	Joback Method
cpg	983.43	J/mol×K	1049.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416628&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

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