Pimelic acid, di(pentafluorobenzyl) ester

Inchi: InChI=1S/C21H14F10O4/c22-12-8(13(23)17(27)20(30)16(12)26)6-34-10(32)4-2-1-3-5-11
InchiKey: XRKNQGOJSWTELL-UHFFFAOYSA-N
Formula: C21H14F10O4
SMILES: O=C(CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 520.32

Physical Properties

Property code	Value	Unit	Source
gf	-2161.48	kJ/mol	Joback Method
hf	-2569.11	kJ/mol	Joback Method
hfus	70.71	kJ/mol	Joback Method
hvap	83.65	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	5.815		Crippen Method
mcvol	291.810	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	928.32	K	Joback Method
tc	1138.98	K	Joback Method
tf	654.69	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.92	J/mol×K	928.32	Joback Method
cpg	910.90	J/mol×K	963.43	Joback Method
cpg	920.65	J/mol×K	998.54	Joback Method
cpg	929.14	J/mol×K	1033.65	Joback Method
cpg	936.37	J/mol×K	1068.76	Joback Method
cpg	942.34	J/mol×K	1103.87	Joback Method
cpg	947.02	J/mol×K	1138.98	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=U416641&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