Pimelic acid, heptyl pentafluorobenzyl ester

Inchi: InChI=1S/C21H27F5O4/c1-2-3-4-5-9-12-29-15(27)10-7-6-8-11-16(28)30-13-14-17(22)19
InchiKey: AACWAMWPFISVOA-UHFFFAOYSA-N
Formula: C21H27F5O4
SMILES: CCCCCCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 438.43

Physical Properties

Property code	Value	Unit	Source
gf	-1251.69	kJ/mol	Joback Method
hf	-1767.74	kJ/mol	Joback Method
hfus	63.22	kJ/mol	Joback Method
hvap	82.15	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	5.889		Crippen Method
mcvol	306.720	ml/mol	McGowan Method
pc	1033.24	kPa	Joback Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook
tb	880.39	K	Joback Method
tc	1077.96	K	Joback Method
tf	562.72	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.71	J/mol×K	880.39	Joback Method
cpg	985.61	J/mol×K	913.32	Joback Method
cpg	999.37	J/mol×K	946.25	Joback Method
cpg	1012.00	J/mol×K	979.17	Joback Method
cpg	1023.50	J/mol×K	1012.10	Joback Method
cpg	1033.88	J/mol×K	1045.03	Joback Method
cpg	1043.15	J/mol×K	1077.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416631&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