Pimelic acid, octyl pentafluorobenzyl ester

Inchi: InChI=1S/C22H29F5O4/c1-2-3-4-5-6-10-13-30-16(28)11-8-7-9-12-17(29)31-14-15-18(23
InchiKey: BNFWYMNNBRRPKB-UHFFFAOYSA-N
Formula: C22H29F5O4
SMILES: CCCCCCCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 452.46

Physical Properties

Property code	Value	Unit	Source
gf	-1243.27	kJ/mol	Joback Method
hf	-1788.38	kJ/mol	Joback Method
hfus	65.81	kJ/mol	Joback Method
hvap	84.38	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.279		Crippen Method
mcvol	320.810	ml/mol	McGowan Method
pc	972.30	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	903.27	K	Joback Method
tc	1106.93	K	Joback Method
tf	573.99	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.47	J/mol×K	903.27	Joback Method
cpg	1045.85	J/mol×K	937.21	Joback Method
cpg	1059.97	J/mol×K	971.16	Joback Method
cpg	1072.85	J/mol×K	1005.10	Joback Method
cpg	1084.49	J/mol×K	1039.05	Joback Method
cpg	1094.92	J/mol×K	1072.99	Joback Method
cpg	1104.13	J/mol×K	1106.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416632&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