Pimelic acid, pentafluorobenzyl undecyl ester

Inchi: InChI=1S/C25H35F5O4/c1-2-3-4-5-6-7-8-9-13-16-33-19(31)14-11-10-12-15-20(32)34-17
InchiKey: YWACDJTYGUZHAF-UHFFFAOYSA-N
Formula: C25H35F5O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 494.54

Physical Properties

Property code	Value	Unit	Source
gf	-1218.01	kJ/mol	Joback Method
hf	-1850.30	kJ/mol	Joback Method
hfus	73.58	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-9.27		Crippen Method
logp	7.450		Crippen Method
mcvol	363.080	ml/mol	McGowan Method
pc	818.66	kPa	Joback Method
rinpol	2952.00		NIST Webbook
rinpol	2952.00		NIST Webbook
tb	971.91	K	Joback Method
tc	1200.48	K	Joback Method
tf	607.80	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.15	J/mol×K	971.91	Joback Method
cpg	1230.03	J/mol×K	1010.01	Joback Method
cpg	1245.20	J/mol×K	1048.10	Joback Method
cpg	1258.69	J/mol×K	1086.20	Joback Method
cpg	1270.52	J/mol×K	1124.29	Joback Method
cpg	1280.73	J/mol×K	1162.39	Joback Method
cpg	1289.35	J/mol×K	1200.48	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=U416635&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