Pimelic acid, pentafluorobenzyl propyl ester

Inchi: InChI=1S/C17H19F5O4/c1-2-8-25-11(23)6-4-3-5-7-12(24)26-9-10-13(18)15(20)17(22)16
InchiKey: CFRNFNDRUISJOU-UHFFFAOYSA-N
Formula: C17H19F5O4
SMILES: CCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 382.32

Physical Properties

Property code	Value	Unit	Source
gf	-1285.37	kJ/mol	Joback Method
hf	-1685.18	kJ/mol	Joback Method
hfus	52.86	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.329		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2073.00		NIST Webbook
rinpol	2073.00		NIST Webbook
tb	788.87	K	Joback Method
tc	971.02	K	Joback Method
tf	517.64	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.11	J/mol×K	788.87	Joback Method
cpg	752.16	J/mol×K	819.23	Joback Method
cpg	764.39	J/mol×K	849.59	Joback Method
cpg	775.81	J/mol×K	879.95	Joback Method
cpg	786.43	J/mol×K	910.31	Joback Method
cpg	796.23	J/mol×K	940.66	Joback Method
cpg	805.22	J/mol×K	971.02	Joback Method

Sources

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=U416625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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