Pimelic acid, hexyl pentafluorobenzyl ester

Inchi: InChI=1S/C20H25F5O4/c1-2-3-4-8-11-28-14(26)9-6-5-7-10-15(27)29-12-13-16(21)18(23
InchiKey: IQVBEGALUKXXTH-UHFFFAOYSA-N
Formula: C20H25F5O4
SMILES: CCCCCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 424.40

Physical Properties

Property code	Value	Unit	Source
gf	-1260.11	kJ/mol	Joback Method
hf	-1747.10	kJ/mol	Joback Method
hfus	60.63	kJ/mol	Joback Method
hvap	79.93	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.499		Crippen Method
mcvol	292.630	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2404.00		NIST Webbook
rinpol	2404.00		NIST Webbook
tb	857.51	K	Joback Method
tc	1049.95	K	Joback Method
tf	551.45	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.62	J/mol×K	857.51	Joback Method
cpg	926.06	J/mol×K	889.58	Joback Method
cpg	939.45	J/mol×K	921.66	Joback Method
cpg	951.81	J/mol×K	953.73	Joback Method
cpg	963.13	J/mol×K	985.80	Joback Method
cpg	973.42	J/mol×K	1017.88	Joback Method
cpg	982.69	J/mol×K	1049.95	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=U416630&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