Pimelic acid, dodecyl pentafluorobenzyl ester

Inchi: InChI=1S/C26H37F5O4/c1-2-3-4-5-6-7-8-9-10-14-17-34-20(32)15-12-11-13-16-21(33)35
InchiKey: RBGZADSOMBVRTL-UHFFFAOYSA-N
Formula: C26H37F5O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 508.56

Physical Properties

Property code	Value	Unit	Source
gf	-1209.59	kJ/mol	Joback Method
hf	-1870.94	kJ/mol	Joback Method
hfus	76.17	kJ/mol	Joback Method
hvap	93.28	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	7.840		Crippen Method
mcvol	377.170	ml/mol	McGowan Method
pc	775.48	kPa	Joback Method
rinpol	2993.00		NIST Webbook
rinpol	2993.00		NIST Webbook
tb	994.79	K	Joback Method
tc	1234.18	K	Joback Method
tf	619.07	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.97	J/mol×K	994.79	Joback Method
cpg	1292.38	J/mol×K	1034.69	Joback Method
cpg	1307.88	J/mol×K	1074.59	Joback Method
cpg	1321.50	J/mol×K	1114.49	Joback Method
cpg	1333.29	J/mol×K	1154.38	Joback Method
cpg	1343.28	J/mol×K	1194.28	Joback Method
cpg	1351.51	J/mol×K	1234.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416636&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