Pimelic acid, decyl pentafluorobenzyl ester

Inchi: InChI=1S/C24H33F5O4/c1-2-3-4-5-6-7-8-12-15-32-18(30)13-10-9-11-14-19(31)33-16-17
InchiKey: XXWMGIPUCOJSRN-UHFFFAOYSA-N
Formula: C24H33F5O4
SMILES: CCCCCCCCCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 480.51

Physical Properties

Property code	Value	Unit	Source
gf	-1226.43	kJ/mol	Joback Method
hf	-1829.66	kJ/mol	Joback Method
hfus	70.99	kJ/mol	Joback Method
hvap	88.83	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	7.060		Crippen Method
mcvol	348.990	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	949.03	K	Joback Method
tc	1168.11	K	Joback Method
tf	596.53	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.76	J/mol×K	949.03	Joback Method
cpg	1168.12	J/mol×K	985.54	Joback Method
cpg	1182.95	J/mol×K	1022.06	Joback Method
cpg	1196.26	J/mol×K	1058.57	Joback Method
cpg	1208.08	J/mol×K	1095.08	Joback Method
cpg	1218.42	J/mol×K	1131.60	Joback Method
cpg	1227.32	J/mol×K	1168.11	Joback Method

Sources

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=U416634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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