Pimelic acid, hexadecyl pentafluorobenzyl ester

Inchi: InChI=1S/C30H45F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-38-24(36)19-16-15-17

InchiKey: FOOUMUWHJFJUSL-UHFFFAOYSA-N

Formula: C30H45F5O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 564.67

Physical Properties

Property code	Value	Unit	Source
gf	-1175.91	kJ/mol	Joback Method
hf	-1953.50	kJ/mol	Joback Method
hfus	86.53	kJ/mol	Joback Method
hvap	102.19	kJ/mol	Joback Method
log10ws	-11.36		Crippen Method
logp	9.400		Crippen Method
mcvol	433.530	ml/mol	McGowan Method
pc	632.89	kPa	Joback Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	1086.31	K	Joback Method
tc	1384.50	K	Joback Method
tf	664.15	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1525.47	J/mol×K	1086.31	Joback Method
cpg	1545.10	J/mol×K	1136.01	Joback Method
cpg	1561.64	J/mol×K	1185.71	Joback Method
cpg	1575.19	J/mol×K	1235.41	Joback Method
cpg	1585.88	J/mol×K	1285.10	Joback Method
cpg	1593.80	J/mol×K	1334.80	Joback Method
cpg	1599.06	J/mol×K	1384.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416640&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

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