Sebacic acid, di(pentafluorophenyl) ester

Inchi: InChI=1S/C22H16F10O4/c23-11-13(25)17(29)21(18(30)14(11)26)35-9(33)7-5-3-1-2-4-6-
InchiKey: DGAJTTIRRZZDGA-UHFFFAOYSA-N
Formula: C22H16F10O4
SMILES: O=C(CCCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 534.34

Physical Properties

Property code	Value	Unit	Source
gf	-2153.06	kJ/mol	Joback Method
hf	-2589.75	kJ/mol	Joback Method
hfus	73.30	kJ/mol	Joback Method
hvap	85.88	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	6.709		Crippen Method
mcvol	305.900	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
rinpol	2411.00		NIST Webbook
tb	951.20	K	Joback Method
tc	1169.85	K	Joback Method
tf	665.96	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.69	J/mol×K	951.20	Joback Method
cpg	969.08	J/mol×K	987.64	Joback Method
cpg	979.06	J/mol×K	1024.08	Joback Method
cpg	987.64	J/mol×K	1060.52	Joback Method
cpg	994.81	J/mol×K	1096.96	Joback Method
cpg	1000.57	J/mol×K	1133.41	Joback Method
cpg	1004.91	J/mol×K	1169.85	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=U355035&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