Sebacic acid, dipentafluorobenzyl ester

Inchi: InChI=1S/C24H20F10O4/c25-15-11(16(26)20(30)23(33)19(15)29)9-37-13(35)7-5-3-1-2-4
InchiKey: PSADLRIMTFQPKD-UHFFFAOYSA-N
Formula: C24H20F10O4
SMILES: O=C(CCCCCCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 562.40

Physical Properties

Property code	Value	Unit	Source
gf	-2136.22	kJ/mol	Joback Method
hf	-2631.03	kJ/mol	Joback Method
hfus	78.48	kJ/mol	Joback Method
hvap	90.33	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	6.985		Crippen Method
mcvol	334.080	ml/mol	McGowan Method
pc	881.57	kPa	Joback Method
rinpol	2731.00		NIST Webbook
tb	996.96	K	Joback Method
tc	1235.29	K	Joback Method
tf	688.50	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.81	J/mol×K	996.96	Joback Method
cpg	1086.92	J/mol×K	1036.68	Joback Method
cpg	1097.26	J/mol×K	1076.40	Joback Method
cpg	1105.82	J/mol×K	1116.13	Joback Method
cpg	1112.60	J/mol×K	1155.85	Joback Method
cpg	1117.61	J/mol×K	1195.57	Joback Method
cpg	1120.85	J/mol×K	1235.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354911&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