Sebacic acid, heptyl pentafluorophenyl ester

Inchi: InChI=1S/C23H31F5O4/c1-2-3-4-9-12-15-31-16(29)13-10-7-5-6-8-11-14-17(30)32-23-21
InchiKey: CWTWOMOXEZBBHO-UHFFFAOYSA-N
Formula: C23H31F5O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 466.48

Physical Properties

Property code	Value	Unit	Source
gf	-1234.85	kJ/mol	Joback Method
hf	-1809.02	kJ/mol	Joback Method
hfus	68.40	kJ/mol	Joback Method
hvap	86.61	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	6.922		Crippen Method
mcvol	334.900	ml/mol	McGowan Method
pc	916.61	kPa	Joback Method
rinpol	2578.00		NIST Webbook
tb	926.15	K	Joback Method
tc	1136.96	K	Joback Method
tf	585.26	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.84	J/mol×K	926.15	Joback Method
cpg	1106.71	J/mol×K	961.28	Joback Method
cpg	1121.19	J/mol×K	996.42	Joback Method
cpg	1134.29	J/mol×K	1031.55	Joback Method
cpg	1146.04	J/mol×K	1066.69	Joback Method
cpg	1156.46	J/mol×K	1101.82	Joback Method
cpg	1165.55	J/mol×K	1136.96	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=U355029&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

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