Sebacic acid, heptyl 2-(pentafluorophenoxy)ethyl ester

Inchi: InChI=1S/C25H35F5O5/c1-2-3-4-9-12-15-33-18(31)13-10-7-5-6-8-11-14-19(32)34-16-17
InchiKey: DHVZURLJAGSYNZ-UHFFFAOYSA-N
Formula: C25H35F5O5
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 510.53

Physical Properties

Property code	Value	Unit	Source
gf	-1323.01	kJ/mol	Joback Method
hf	-1982.52	kJ/mol	Joback Method
hfus	74.76	kJ/mol	Joback Method
hvap	93.47	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	6.938		Crippen Method
mcvol	368.950	ml/mol	McGowan Method
pc	810.76	kPa	Joback Method
rinpol	2788.00		NIST Webbook
rinpol	2788.00		NIST Webbook
tb	994.33	K	Joback Method
tc	1232.95	K	Joback Method
tf	630.03	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1241.83	J/mol×K	994.33	Joback Method
cpg	1258.07	J/mol×K	1034.10	Joback Method
cpg	1272.28	J/mol×K	1073.87	Joback Method
cpg	1284.47	J/mol×K	1113.64	Joback Method
cpg	1294.65	J/mol×K	1153.41	Joback Method
cpg	1302.85	J/mol×K	1193.18	Joback Method
cpg	1309.06	J/mol×K	1232.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416785&Units=SI

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