Sebacic acid, hexyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C21H32F8O4/c1-2-3-4-11-14-32-16(30)12-9-7-5-6-8-10-13-17(31)33-15-19(24
InchiKey: MQPWDHUQOFKIFV-UHFFFAOYSA-N
Formula: C21H32F8O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 500.46

Physical Properties

Property code	Value	Unit	Source
gf	-1894.30	kJ/mol	Joback Method
hf	-2566.78	kJ/mol	Joback Method
hfus	54.59	kJ/mol	Joback Method
hvap	69.84	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.945		Crippen Method
mcvol	335.790	ml/mol	McGowan Method
pc	846.53	kPa	Joback Method
rinpol	2252.00		NIST Webbook
rinpol	2252.00		NIST Webbook
tb	816.49	K	Joback Method
tc	1000.80	K	Joback Method
tf	467.73	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.24	J/mol×K	816.49	Joback Method
cpg	1109.25	J/mol×K	847.21	Joback Method
cpg	1125.20	J/mol×K	877.93	Joback Method
cpg	1140.14	J/mol×K	908.64	Joback Method
cpg	1154.15	J/mol×K	939.36	Joback Method
cpg	1167.28	J/mol×K	970.08	Joback Method
cpg	1179.59	J/mol×K	1000.80	Joback Method

Sources

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=U355738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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