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

Inchi: InChI=1S/C21H32F8O4/c1-15(2)10-9-13-32-16(30)11-7-5-3-4-6-8-12-17(31)33-14-19(24
InchiKey: RTCFRBCTZQIFDT-UHFFFAOYSA-N
Formula: C21H32F8O4
SMILES: CC(C)CCCOC(=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	-1896.74	kJ/mol	Joback Method
hf	-2572.06	kJ/mol	Joback Method
hfus	51.07	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.801		Crippen Method
mcvol	335.790	ml/mol	McGowan Method
pc	850.48	kPa	Joback Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	816.05	K	Joback Method
tc	999.77	K	Joback Method
tf	452.73	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.73	J/mol×K	816.05	Joback Method
cpg	1109.70	J/mol×K	846.67	Joback Method
cpg	1125.59	J/mol×K	877.29	Joback Method
cpg	1140.48	J/mol×K	907.91	Joback Method
cpg	1154.42	J/mol×K	938.53	Joback Method
cpg	1167.48	J/mol×K	969.15	Joback Method
cpg	1179.73	J/mol×K	999.77	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=U355737&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