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

Inchi: InChI=1S/C19H28F8O4/c1-13(2)11-30-14(28)9-7-5-3-4-6-8-10-15(29)31-12-17(22,23)19

InchiKey: FCZXNMURSXVHFT-UHFFFAOYSA-N

Formula: C19H28F8O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 472.41

Physical Properties

Property code	Value	Unit	Source
gf	-1913.58	kJ/mol	Joback Method
hf	-2530.78	kJ/mol	Joback Method
hfus	45.89	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	6.021		Crippen Method
mcvol	307.610	ml/mol	McGowan Method
pc	954.37	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	770.29	K	Joback Method
tc	943.28	K	Joback Method
tf	430.19	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.39	J/mol×K	770.29	Joback Method
cpg	990.19	J/mol×K	799.12	Joback Method
cpg	1005.04	J/mol×K	827.95	Joback Method
cpg	1018.99	J/mol×K	856.78	Joback Method
cpg	1032.09	J/mol×K	885.61	Joback Method
cpg	1044.38	J/mol×K	914.45	Joback Method
cpg	1055.93	J/mol×K	943.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355734&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

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