Sebacic acid, di(2,2,3,3,4,4,5,5-octafluoropentyl) ester

Inchi: InChI=1S/C20H22F16O4/c21-13(22)17(29,30)19(33,34)15(25,26)9-39-11(37)7-5-3-1-2-4

InchiKey: SDVCVWKENPHZSW-UHFFFAOYSA-N

Formula: C20H22F16O4

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

Mol. weight [g/mol]: 630.36

Physical Properties

Property code	Value	Unit	Source
gf	-3455.12	kJ/mol	Joback Method
hf	-4146.55	kJ/mol	Joback Method
hfus	50.88	kJ/mol	Joback Method
hvap	56.80	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.536		Crippen Method
mcvol	335.860	ml/mol	McGowan Method
pc	756.40	kPa	Joback Method
rinpol	1983.00		NIST Webbook
tb	777.64	K	Joback Method
tc	957.26	K	Joback Method
tf	453.44	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.83	J/mol×K	777.64	Joback Method
cpg	1113.04	J/mol×K	807.58	Joback Method
cpg	1127.16	J/mol×K	837.51	Joback Method
cpg	1140.29	J/mol×K	867.45	Joback Method
cpg	1152.54	J/mol×K	897.39	Joback Method
cpg	1164.01	J/mol×K	927.33	Joback Method
cpg	1174.80	J/mol×K	957.26	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=U355751&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