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

Inchi: InChI=1S/C22H34F8O4/c1-2-3-4-9-12-15-33-17(31)13-10-7-5-6-8-11-14-18(32)34-16-20

InchiKey: BVBUCFQUXMWHSP-UHFFFAOYSA-N

Formula: C22H34F8O4

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

Mol. weight [g/mol]: 514.49

Physical Properties

Property code	Value	Unit	Source
gf	-1885.88	kJ/mol	Joback Method
hf	-2587.42	kJ/mol	Joback Method
hfus	57.18	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	7.335		Crippen Method
mcvol	349.880	ml/mol	McGowan Method
pc	801.15	kPa	Joback Method
rinpol	2343.00		NIST Webbook
rinpol	2343.00		NIST Webbook
tb	839.37	K	Joback Method
tc	1030.78	K	Joback Method
tf	479.00	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.56	J/mol×K	839.37	Joback Method
cpg	1170.27	J/mol×K	871.27	Joback Method
cpg	1186.84	J/mol×K	903.17	Joback Method
cpg	1202.33	J/mol×K	935.07	Joback Method
cpg	1216.83	J/mol×K	966.98	Joback Method
cpg	1230.41	J/mol×K	998.88	Joback Method
cpg	1243.15	J/mol×K	1030.78	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=U355739&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