Succinic acid, 2,2,3,3,4,4,4-heptafluorobutyl hexadecyl ester

Inchi: InChI=1S/C24H39F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-34-20(32)16-17-21(33

InchiKey: BRIKPZVAWMXZAY-UHFFFAOYSA-N

Formula: C24H39F7O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 524.55

Physical Properties

Property code	Value	Unit	Source
gf	-1671.79	kJ/mol	Joback Method
hf	-2427.31	kJ/mol	Joback Method
hfus	62.81	kJ/mol	Joback Method
hvap	77.72	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.167		Crippen Method
mcvol	376.290	ml/mol	McGowan Method
pc	735.22	kPa	Joback Method
rinpol	2425.00		NIST Webbook
rinpol	2425.00		NIST Webbook
tb	886.30	K	Joback Method
tc	1093.48	K	Joback Method
tf	515.95	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1267.64	J/mol×K	886.30	Joback Method
cpg	1286.94	J/mol×K	920.83	Joback Method
cpg	1304.94	J/mol×K	955.36	Joback Method
cpg	1321.74	J/mol×K	989.89	Joback Method
cpg	1337.45	J/mol×K	1024.42	Joback Method
cpg	1352.15	J/mol×K	1058.95	Joback Method
cpg	1365.96	J/mol×K	1093.48	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=U382363&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