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

Inchi: InChI=1S/C19H29F7O4/c1-2-3-4-5-6-7-8-9-10-13-29-15(27)11-12-16(28)30-14-17(20,21)

InchiKey: DZWFAPWHPIFROZ-UHFFFAOYSA-N

Formula: C19H29F7O4

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

Mol. weight [g/mol]: 454.42

Physical Properties

Property code	Value	Unit	Source
gf	-1713.89	kJ/mol	Joback Method
hf	-2324.11	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.217		Crippen Method
mcvol	305.840	ml/mol	McGowan Method
pc	971.70	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
tb	771.90	K	Joback Method
tc	945.29	K	Joback Method
tf	459.60	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.81	J/mol×K	771.90	Joback Method
cpg	981.70	J/mol×K	800.80	Joback Method
cpg	996.65	J/mol×K	829.70	Joback Method
cpg	1010.73	J/mol×K	858.60	Joback Method
cpg	1023.97	J/mol×K	887.50	Joback Method
cpg	1036.42	J/mol×K	916.39	Joback Method
cpg	1048.14	J/mol×K	945.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382358&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