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

Inchi: InChI=1S/C21H33F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-31-17(29)13-14-18(30)32-16-19

InchiKey: RFNDAJAYOJEQNL-UHFFFAOYSA-N

Formula: C21H33F7O4

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

Mol. weight [g/mol]: 482.47

Physical Properties

Property code	Value	Unit	Source
gf	-1697.05	kJ/mol	Joback Method
hf	-2365.39	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	71.05	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.997		Crippen Method
mcvol	334.020	ml/mol	McGowan Method
pc	865.05	kPa	Joback Method
rinpol	2147.00		NIST Webbook
rinpol	2147.00		NIST Webbook
tb	817.66	K	Joback Method
tc	1001.67	K	Joback Method
tf	482.14	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.34	J/mol×K	817.66	Joback Method
cpg	1101.42	J/mol×K	848.33	Joback Method
cpg	1117.45	J/mol×K	879.00	Joback Method
cpg	1132.49	J/mol×K	909.66	Joback Method
cpg	1146.61	J/mol×K	940.33	Joback Method
cpg	1159.87	J/mol×K	971.00	Joback Method
cpg	1172.33	J/mol×K	1001.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382360&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