Succinic acid, dodec-2-en-1-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C20H30F6O4/c1-2-3-4-5-6-7-8-9-10-11-14-29-16(27)12-13-17(28)30-15-19(22

InchiKey: XEOVTQNLYPUGJI-ZHACJKMWSA-N

Formula: C20H30F6O4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)OCC(F)(F)C(F)C(F)(F)F

Mol. weight [g/mol]: 448.44

Physical Properties

Property code	Value	Unit	Source
gf	-1435.72	kJ/mol	Joback Method
hf	-2027.95	kJ/mol	Joback Method
hfus	53.46	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.086		Crippen Method
mcvol	313.860	ml/mol	McGowan Method
pc	965.67	kPa	Joback Method
rinpol	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	802.46	K	Joback Method
tc	982.55	K	Joback Method
tf	447.78	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.26	J/mol×K	802.46	Joback Method
cpg	1007.40	J/mol×K	832.48	Joback Method
cpg	1022.58	J/mol×K	862.49	Joback Method
cpg	1036.87	J/mol×K	892.51	Joback Method
cpg	1050.32	J/mol×K	922.52	Joback Method
cpg	1062.97	J/mol×K	952.54	Joback Method
cpg	1074.89	J/mol×K	982.55	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=U390814&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