Succinic acid, 2,2,3,3-tetrafluoropropyl cis-hex-3-en-1-yl ester

Inchi: InChI=1S/C13H18F4O4/c1-2-3-4-5-8-20-10(18)6-7-11(19)21-9-13(16,17)12(14)15/h3-4,1

InchiKey: XMOSVRDEDQSNDQ-ARJAWSKDSA-N

Formula: C13H18F4O4

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

Mol. weight [g/mol]: 314.27

Physical Properties

Property code	Value	Unit	Source
gf	-1107.88	kJ/mol	Joback Method
hf	-1482.50	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.110		Crippen Method
mcvol	211.690	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
tb	646.99	K	Joback Method
tc	815.19	K	Joback Method
tf	365.29	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.24	J/mol×K	646.99	Joback Method
cpg	595.47	J/mol×K	675.02	Joback Method
cpg	608.02	J/mol×K	703.06	Joback Method
cpg	619.91	J/mol×K	731.09	Joback Method
cpg	631.17	J/mol×K	759.12	Joback Method
cpg	641.81	J/mol×K	787.15	Joback Method
cpg	651.86	J/mol×K	815.19	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=U391080&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