Succinic acid, 2,2,3,3-tetrafluoropropyl 3-methylpentyl ester

Inchi: InChI=1S/C13H20F4O4/c1-3-9(2)6-7-20-10(18)4-5-11(19)21-8-13(16,17)12(14)15/h9,12H

InchiKey: KRURQLMBPGKGOO-UHFFFAOYSA-N

Formula: C13H20F4O4

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

Mol. weight [g/mol]: 316.29

Physical Properties

Property code	Value	Unit	Source
gf	-1190.54	kJ/mol	Joback Method
hf	-1605.00	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.190		Crippen Method
mcvol	215.990	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	642.39	K	Joback Method
tc	807.96	K	Joback Method
tf	355.37	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.03	J/mol×K	642.39	Joback Method
cpg	617.98	J/mol×K	669.98	Joback Method
cpg	631.26	J/mol×K	697.58	Joback Method
cpg	643.86	J/mol×K	725.17	Joback Method
cpg	655.81	J/mol×K	752.77	Joback Method
cpg	667.12	J/mol×K	780.36	Joback Method
cpg	677.80	J/mol×K	807.96	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=U390638&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