Succinic acid, 3-methylbut-2-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C12H17F5O4/c1-7(2)8(3)21-10(19)5-4-9(18)20-6-11(13,14)12(15,16)17/h7-8H

InchiKey: BPTZAEMSNFQMBZ-UHFFFAOYSA-N

Formula: C12H17F5O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 320.25

Physical Properties

Property code	Value	Unit	Source
gf	-1390.93	kJ/mol	Joback Method
hf	-1789.22	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	53.16	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.095		Crippen Method
mcvol	203.670	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook
tb	615.55	K	Joback Method
tc	781.99	K	Joback Method
tf	347.11	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.15	J/mol×K	615.55	Joback Method
cpg	576.53	J/mol×K	643.29	Joback Method
cpg	589.20	J/mol×K	671.03	Joback Method
cpg	601.18	J/mol×K	698.77	Joback Method
cpg	612.48	J/mol×K	726.51	Joback Method
cpg	623.14	J/mol×K	754.25	Joback Method
cpg	633.18	J/mol×K	781.99	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=U390861&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