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

Inchi: InChI=1S/C12H18F4O4/c1-7(2)8(3)20-10(18)5-4-9(17)19-6-12(15,16)11(13)14/h7-8,11H

InchiKey: UFYLEJSKAZWDQF-UHFFFAOYSA-N

Formula: C12H18F4O4

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

Mol. weight [g/mol]: 302.26

Physical Properties

Property code	Value	Unit	Source
gf	-1201.40	kJ/mol	Joback Method
hf	-1589.64	kJ/mol	Joback Method
hfus	26.75	kJ/mol	Joback Method
hvap	54.89	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.798		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1372.00		NIST Webbook
rinpol	1372.00		NIST Webbook
tb	619.07	K	Joback Method
tc	786.95	K	Joback Method
tf	329.10	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.45	J/mol×K	619.07	Joback Method
cpg	566.10	J/mol×K	647.05	Joback Method
cpg	579.07	J/mol×K	675.03	Joback Method
cpg	591.39	J/mol×K	703.01	Joback Method
cpg	603.06	J/mol×K	730.99	Joback Method
cpg	614.10	J/mol×K	758.97	Joback Method
cpg	624.52	J/mol×K	786.95	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=U390578&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