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

Inchi: InChI=1S/C13H20F4O4/c1-8(12(2,3)4)21-10(19)6-5-9(18)20-7-13(16,17)11(14)15/h8,11H

InchiKey: BHLQPGNURDCGQD-UHFFFAOYSA-N

Formula: C13H20F4O4

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

Mol. weight [g/mol]: 316.29

Physical Properties

Property code	Value	Unit	Source
gf	-1187.70	kJ/mol	Joback Method
hf	-1613.75	kJ/mol	Joback Method
hfus	25.45	kJ/mol	Joback Method
hvap	56.21	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.188		Crippen Method
mcvol	215.990	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1419.00		NIST Webbook
rinpol	1419.00		NIST Webbook
tb	639.16	K	Joback Method
tc	810.93	K	Joback Method
tf	357.79	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.89	J/mol×K	639.16	Joback Method
cpg	621.26	J/mol×K	667.79	Joback Method
cpg	634.84	J/mol×K	696.42	Joback Method
cpg	647.66	J/mol×K	725.05	Joback Method
cpg	659.76	J/mol×K	753.68	Joback Method
cpg	671.15	J/mol×K	782.30	Joback Method
cpg	681.86	J/mol×K	810.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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