

Succinic acid, 2,2,3,3-tetrafluoropropyl but-2-en-1-yl ester

Inchi: InChI=1S/C11H14F4O4/c1-2-3-6-18-8(16)4-5-9(17)19-7-11(14,15)10(12)13/h2-3,10H,4-7
InchiKey: IFNYRDFNZPRDQJ-NSCUHMNNSA-N
Formula: C11H14F4O4
SMILES: CC=CCOC(=O)CCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 286.22

Physical Properties

Property code	Value	Unit	Source
gf	-1124.72	kJ/mol	Joback Method
hf	-1441.22	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	53.40	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.329		Crippen Method
mcvol	183.510	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
tb	601.23	K	Joback Method
tc	770.07	K	Joback Method
tf	342.75	K	Joback Method
vc	0.735	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.89	J/molxK	601.23	Joback Method
cpg	492.98	J/molxK	629.37	Joback Method
cpg	504.45	J/molxK	657.51	Joback Method
cpg	515.33	J/molxK	685.65	Joback Method
cpg	525.62	J/molxK	713.79	Joback Method
cpg	535.36	J/molxK	741.93	Joback Method
cpg	544.55	J/molxK	770.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U391218&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/117-947-1/Succinic-acid-2-2-3-3-tetrafluoropropyl-but-2-en-1-yl-ester.pdf>

Generated by Cheméo on 2024-04-30 00:05:34.239163031 +0000 UTC m=+16724783.159740352.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.