

Succinic acid, 1,1,1-trifluoroprop-2-yl dec-9-en-1-yl ester

Inchi:	InChI=1S/C17H27F3O4/c1-3-4-5-6-7-8-9-10-13-23-15(21)11-12-16(22)24-14(2)17(18,19
InchiKey:	MRRJMYLQYGYRBD-UHFFFAOYSA-N
Formula:	C17H27F3O4
SMILES:	C=CCCCCCCCCOC(=O)CCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]:	352.39

Physical Properties

Property code	Value	Unit	Source
gf	-871.77	kJ/mol	Joback Method
hf	-1360.74	kJ/mol	Joback Method
hfus	42.38	kJ/mol	Joback Method
hvap	66.94	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.721		Crippen Method
mcvol	266.280	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	731.76	K	Joback Method
tc	904.69	K	Joback Method
tf	413.10	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.39	J/molxK	731.76	Joback Method
cpg	806.94	J/molxK	760.58	Joback Method
cpg	821.66	J/molxK	789.40	Joback Method
cpg	835.57	J/molxK	818.23	Joback Method
cpg	848.69	J/molxK	847.05	Joback Method
cpg	861.04	J/molxK	875.87	Joback Method
cpg	872.66	J/molxK	904.69	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=U391245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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