

Succinic acid, ethyl pent-4-en-2-yl ester

Inchi:	InChI=1S/C11H18O4/c1-4-6-9(3)15-11(13)8-7-10(12)14-5-2/h4,9H,1,5-8H2,2-3H3
InchiKey:	PFLRZSGVXOTHLU-UHFFFAOYSA-N
Formula:	C11H18O4
SMILES:	C=CCC(C)OC(=O)CCC(=O)OCC
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
gf	-340.70	kJ/mol	Joback Method
hf	-639.82	kJ/mol	Joback Method
hfus	25.02	kJ/mol	Joback Method
hvap	57.33	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.837		Crippen Method
mcvol	176.430	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1393.00		NIST Webbook
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tb	599.90	K	Joback Method
tc	784.60	K	Joback Method
tf	341.29	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.35	J/mol×K	599.90	Joback Method
cpg	506.32	J/mol×K	753.82	Joback Method
cpg	495.15	J/mol×K	723.03	Joback Method
cpg	483.37	J/mol×K	692.25	Joback Method
cpg	470.98	J/mol×K	661.47	Joback Method
cpg	457.97	J/mol×K	630.68	Joback Method
cpg	516.88	J/mol×K	784.60	Joback Method
dvisc	0.0001652	Pa×s	599.90	Joback Method

dvisc	0.0002153	Pa×s	556.80	Joback Method
dvisc	0.0002935	Pa×s	513.70	Joback Method
dvisc	0.0004234	Pa×s	470.60	Joback Method
dvisc	0.0006577	Pa×s	427.49	Joback Method
dvisc	0.0011277	Pa×s	384.39	Joback Method
dvisc	0.0022154	Pa×s	341.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353457&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
dvisc:	Dynamic viscosity
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

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