

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

Inchi:	InChI=1S/C9H13ClO3/c1-3-4-7(2)13-9(12)6-5-8(10)11/h3,7H,1,4-6H2,2H3
InchiKey:	LBRRWHKGDPAWTB-UHFFFAOYSA-N
Formula:	C9H13ClO3
SMILES:	C=CCC(C)OC(=O)CCC(=O)Cl
Mol. weight [g/mol]:	204.65

Physical Properties

Property code	Value	Unit	Source
gf	-264.47	kJ/mol	Joback Method
hf	-482.06	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	54.86	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.040		Crippen Method
mvol	154.620	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1275.00		NIST Webbook
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tb	569.15	K	Joback Method
tc	763.87	K	Joback Method
tf	326.44	K	Joback Method
vc	0.594	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.08	J/molxK	569.15	Joback Method
cpg	362.66	J/molxK	601.60	Joback Method
cpg	373.65	J/molxK	634.06	Joback Method
cpg	384.07	J/molxK	666.51	Joback Method
cpg	393.93	J/molxK	698.96	Joback Method
cpg	403.24	J/molxK	731.42	Joback Method
cpg	412.01	J/molxK	763.87	Joback Method
dvisc	0.0029667	Paxs	326.44	Joback Method

dvisc	0.0015530	Paxs	366.89	Joback Method
dvisc	0.0009245	Paxs	407.34	Joback Method
dvisc	0.0006044	Paxs	447.79	Joback Method
dvisc	0.0004240	Paxs	488.25	Joback Method
dvisc	0.0003140	Paxs	528.70	Joback Method
dvisc	0.0002427	Paxs	569.15	Joback Method

Sources

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=U353459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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