

Succinic acid, 2-chloropropyl ethyl ester

Inchi: InChI=1S/C9H15ClO4/c1-3-13-8(11)4-5-9(12)14-6-7(2)10/h7H,3-6H2,1-2H3
InchiKey: JBPBSXHYWSBZCF-UHFFFAOYSA-N
Formula: C9H15ClO4
SMILES: CCOC(=O)CCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 222.67

Physical Properties

Property code	Value	Unit	Source
gf	-457.31	kJ/mol	Joback Method
hf	-739.71	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.500		Crippen Method
mvol	164.790	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	1457.00		NIST Webbook
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tb	594.89	K	Joback Method
tc	784.66	K	Joback Method
tf	350.43	K	Joback Method
vc	0.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.30	J/mol×K	594.89	Joback Method
cpg	407.39	J/mol×K	626.52	Joback Method
cpg	418.93	J/mol×K	658.15	Joback Method
cpg	429.91	J/mol×K	689.78	Joback Method
cpg	440.35	J/mol×K	721.41	Joback Method
cpg	450.22	J/mol×K	753.04	Joback Method
cpg	459.52	J/mol×K	784.66	Joback Method
dvisc	0.0021843	Paxs	350.43	Joback Method

dvisc	0.0011689	Paxs	391.17	Joback Method
dvisc	0.0007038	Paxs	431.92	Joback Method
dvisc	0.0004625	Paxs	472.66	Joback Method
dvisc	0.0003249	Paxs	513.40	Joback Method
dvisc	0.0002404	Paxs	554.15	Joback Method
dvisc	0.0001854	Paxs	594.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349369&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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