

Succinic acid, monochloride, 4-methylpent-2-yl ester

Inchi:	InChI=1S/C10H17ClO3/c1-7(2)6-8(3)14-10(13)5-4-9(11)12/h7-8H,4-6H2,1-3H3
InchiKey:	OEDRJAVMOAYALV-UHFFFAOYSA-N
Formula:	C10H17ClO3
SMILES:	CC(C)CC(C)OC(=O)CCC(=O)Cl
Mol. weight [g/mol]:	220.69

Physical Properties

Property code	Value	Unit	Source
gf	-346.33	kJ/mol	Joback Method
hf	-633.41	kJ/mol	Joback Method
hfus	23.19	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.510		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1327.00		NIST Webbook
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tb	594.91	K	Joback Method
tc	787.34	K	Joback Method
tf	324.47	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.12	J/mol×K	594.91	Joback Method
cpg	479.10	J/mol×K	755.26	Joback Method
cpg	468.38	J/mol×K	723.19	Joback Method
cpg	457.03	J/mol×K	691.12	Joback Method
cpg	445.04	J/mol×K	659.05	Joback Method
cpg	432.41	J/mol×K	626.98	Joback Method
cpg	489.20	J/mol×K	787.34	Joback Method
dvisc	0.0001969	Pa×s	594.91	Joback Method

dvisc	0.0002635	Pa×s	549.84	Joback Method
dvisc	0.0003714	Pa×s	504.76	Joback Method
dvisc	0.0005600	Pa×s	459.69	Joback Method
dvisc	0.0009231	Pa×s	414.62	Joback Method
dvisc	0.0017189	Pa×s	369.54	Joback Method
dvisc	0.0038044	Pa×s	324.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349240&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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