Succinic acid, monochloride, 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C11H19ClO3/c1-7(2)11(8(3)4)15-10(14)6-5-9(12)13/h7-8,11H,5-6H2,1-4H3
InchiKey: LQAKEJMUFGKWGB-UHFFFAOYSA-N
Formula: C11H19ClO3
SMILES: CC(C)C(OC(=O)CCC(=O)Cl)C(C)C
Mol. weight [g/mol]: 234.72

Physical Properties

Property code	Value	Unit	Source
gf	-340.35	kJ/mol	Joback Method
hf	-659.33	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	59.20	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.756		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1431.00		NIST Webbook
rinpol	1431.00		NIST Webbook
tb	617.35	K	Joback Method
tc	811.02	K	Joback Method
tf	320.74	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.93	J/mol×K	617.35	Joback Method
cpg	483.18	J/mol×K	649.63	Joback Method
cpg	496.71	J/mol×K	681.91	Joback Method
cpg	509.51	J/mol×K	714.18	Joback Method
cpg	521.61	J/mol×K	746.46	Joback Method
cpg	533.01	J/mol×K	778.74	Joback Method
cpg	543.72	J/mol×K	811.02	Joback Method
dvisc	0.0047209	Pa×s	320.74	Joback Method

dvisc	0.0018535	Pa×s	370.18	Joback Method
dvisc	0.0009070	Pa×s	419.61	Joback Method
dvisc	0.0005160	Pa×s	469.05	Joback Method
dvisc	0.0003269	Pa×s	518.48	Joback Method
dvisc	0.0002243	Pa×s	567.91	Joback Method
dvisc	0.0001634	Pa×s	617.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349368&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