Succinic acid, 7-chloroheptyl ethyl ester

Inchi: InChI=1S/C13H23ClO4/c1-2-17-12(15)8-9-13(16)18-11-7-5-3-4-6-10-14/h2-11H2,1H3
InchiKey: BAZDIWBYDNMQPS-UHFFFAOYSA-N
Formula: C13H23ClO4
SMILES: CCOC(=O)CCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 278.77

Physical Properties

Property code	Value	Unit	Source
gf	-421.19	kJ/mol	Joback Method
hf	-816.99	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.062		Crippen Method
mcvol	221.150	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	686.85	K	Joback Method
tc	867.86	K	Joback Method
tf	410.51	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.34	J/mol×K	686.85	Joback Method
cpg	612.70	J/mol×K	717.02	Joback Method
cpg	626.35	J/mol×K	747.19	Joback Method
cpg	639.30	J/mol×K	777.35	Joback Method
cpg	651.53	J/mol×K	807.52	Joback Method
cpg	663.07	J/mol×K	837.69	Joback Method
cpg	673.92	J/mol×K	867.86	Joback Method
dvisc	0.0013375	Pa×s	410.51	Joback Method

dvisc	0.0007339	Pa×s	456.57	Joback Method
dvisc	0.0004495	Pa×s	502.62	Joback Method
dvisc	0.0002990	Pa×s	548.68	Joback Method
dvisc	0.0002118	Pa×s	594.74	Joback Method
dvisc	0.0001577	Pa×s	640.79	Joback Method
dvisc	0.0001221	Pa×s	686.85	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=U382410&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