Succinic acid, 10-chlorodecyl undecyl ester

Inchi: InChI=1S/C25H47ClO4/c1-2-3-4-5-6-8-11-14-17-22-29-24(27)19-20-25(28)30-23-18-15-1
InchiKey: ARTWONRGYWKMRD-UHFFFAOYSA-N
Formula: C25H47ClO4
SMILES: CCCCCCCCCCCOC(=O)CCC(=O)OCCCCCCCCCCCl
Mol. weight [g/mol]: 447.09

Physical Properties

Property code	Value	Unit	Source
gf	-320.15	kJ/mol	Joback Method
hf	-1064.67	kJ/mol	Joback Method
hfus	70.28	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	7.743		Crippen Method
mcvol	390.230	ml/mol	McGowan Method
pc	787.71	kPa	Joback Method
rinpol	3149.00		NIST Webbook
rinpol	3149.00		NIST Webbook
tb	961.41	K	Joback Method
tc	1183.64	K	Joback Method
tf	545.75	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.77	J/mol×K	961.41	Joback Method
cpg	1331.62	J/mol×K	998.45	Joback Method
cpg	1349.83	J/mol×K	1035.49	Joback Method
cpg	1366.46	J/mol×K	1072.52	Joback Method
cpg	1381.56	J/mol×K	1109.56	Joback Method
cpg	1395.18	J/mol×K	1146.60	Joback Method
cpg	1407.37	J/mol×K	1183.64	Joback Method
dvisc	0.0003575	Pa×s	545.75	Joback Method

dvisc	0.0001710	Pa×s	615.03	Joback Method
dvisc	0.0000950	Pa×s	684.30	Joback Method
dvisc	0.0000588	Pa×s	753.58	Joback Method
dvisc	0.0000394	Pa×s	822.86	Joback Method
dvisc	0.0000281	Pa×s	892.13	Joback Method
dvisc	0.0000211	Pa×s	961.41	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=U349192&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