Succinic acid, 3-chlorophenethyl octadecyl ester

Inchi: InChI=1S/C30H49ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-34-29(32)21-22-
InchiKey: QFAGLVBQMQZBMU-UHFFFAOYSA-N
Formula: C30H49ClO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1cccc(Cl)c1
Mol. weight [g/mol]: 509.16

Physical Properties

Property code	Value	Unit	Source
gf	-175.27	kJ/mol	Joback Method
hf	-942.81	kJ/mol	Joback Method
hfus	76.88	kJ/mol	Joback Method
hvap	108.01	kJ/mol	Joback Method
log10ws	-9.89		Crippen Method
logp	9.011		Crippen Method
mcvol	436.920	ml/mol	McGowan Method
pc	719.91	kPa	Joback Method
rinpol	3654.00		NIST Webbook
rinpol	3654.00		NIST Webbook
tb	1107.47	K	Joback Method
tc	1376.24	K	Joback Method
tf	641.04	K	Joback Method
vc	1.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.36	J/mol×K	1107.47	Joback Method
cpg	1539.23	J/mol×K	1152.27	Joback Method
cpg	1554.91	J/mol×K	1197.06	Joback Method
cpg	1568.52	J/mol×K	1241.86	Joback Method
cpg	1580.19	J/mol×K	1286.65	Joback Method
cpg	1590.03	J/mol×K	1331.45	Joback Method
cpg	1598.18	J/mol×K	1376.24	Joback Method
dvisc	0.0001423	Pa×s	641.04	Joback Method

dvisc	0.0000721	Pa×s	718.78	Joback Method
dvisc	0.0000418	Pa×s	796.52	Joback Method
dvisc	0.0000266	Pa×s	874.25	Joback Method
dvisc	0.0000183	Pa×s	951.99	Joback Method
dvisc	0.0000133	Pa×s	1029.73	Joback Method
dvisc	0.0000101	Pa×s	1107.47	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=U381509&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