Succinic acid, 4-chloro-3-methylphenyl but-3-en-1-yl ester

Inchi: InChI=1S/C15H17ClO4/c1-3-4-9-19-14(17)7-8-15(18)20-12-5-6-13(16)11(2)10-12/h3,5-6

InchiKey: NCHKAOKOADHIRM-UHFFFAOYSA-N

Formula: C15H17ClO4

SMILES: C=CCCOC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-223.36	kJ/mol	Joback Method
hf	-519.25	kJ/mol	Joback Method
hfus	36.36	kJ/mol	Joback Method
hvap	74.61	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.453		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	765.93	K	Joback Method
tc	976.90	K	Joback Method
tf	482.75	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.68	J/mol×K	765.93	Joback Method
cpg	606.71	J/mol×K	801.09	Joback Method
cpg	618.82	J/mol×K	836.25	Joback Method
cpg	630.02	J/mol×K	871.41	Joback Method
cpg	640.31	J/mol×K	906.57	Joback Method
cpg	649.72	J/mol×K	941.73	Joback Method
cpg	658.25	J/mol×K	976.90	Joback Method
dvisc	0.0006825	Pa×s	482.75	Joback Method

dvisc	0.0004306	Pa×s	529.95	Joback Method
dvisc	0.0002929	Pa×s	577.14	Joback Method
dvisc	0.0002112	Pa×s	624.34	Joback Method
dvisc	0.0001595	Pa×s	671.54	Joback Method
dvisc	0.0001249	Pa×s	718.73	Joback Method
dvisc	0.0001009	Pa×s	765.93	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=U391199&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