Succinic acid, 2-chloro-5-methylphenyl propyl ester

Inchi: InChI=1S/C14H17ClO4/c1-3-8-18-13(16)6-7-14(17)19-12-9-10(2)4-5-11(12)15/h4-5,9H,3

InchiKey: RRWOALHXBNYCKL-UHFFFAOYSA-N

Formula: C14H17ClO4

SMILES: CCCOC(=O)CCC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 284.74

Physical Properties

Property code	Value	Unit	Source
gf	-319.62	kJ/mol	Joback Method
hf	-624.04	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	73.05	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.287		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2010.00		NIST Webbook
tb	746.37	K	Joback Method
tc	956.53	K	Joback Method
tf	473.24	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.84	J/mol×K	746.37	Joback Method
cpg	578.06	J/mol×K	781.40	Joback Method
cpg	590.37	J/mol×K	816.42	Joback Method
cpg	601.78	J/mol×K	851.45	Joback Method
cpg	612.31	J/mol×K	886.48	Joback Method
cpg	621.94	J/mol×K	921.51	Joback Method
cpg	630.68	J/mol×K	956.53	Joback Method
dvisc	0.0007271	Pa×s	473.24	Joback Method
dvisc	0.0004601	Pa×s	518.76	Joback Method

dvisc	0.0003135	Pa×s	564.28	Joback Method
dvisc	0.0002262	Pa×s	609.81	Joback Method
dvisc	0.0001708	Pa×s	655.33	Joback Method
dvisc	0.0001337	Pa×s	700.85	Joback Method
dvisc	0.0001079	Pa×s	746.37	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=U353613&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