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

Inchi: InChI=1S/C18H25ClO4/c1-3-4-5-6-7-12-22-17(20)10-11-18(21)23-16-13-14(2)8-9-15(16)

InchiKey: UGNBFLNKDMWTCH-UHFFFAOYSA-N

Formula: C18H25ClO4

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

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-285.94	kJ/mol	Joback Method
hf	-706.60	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.848		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	837.89	K	Joback Method
tc	1042.84	K	Joback Method
tf	518.32	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.46	J/mol×K	837.89	Joback Method
cpg	801.91	J/mol×K	872.05	Joback Method
cpg	815.29	J/mol×K	906.21	Joback Method
cpg	827.62	J/mol×K	940.37	Joback Method
cpg	838.91	J/mol×K	974.53	Joback Method
cpg	849.18	J/mol×K	1008.69	Joback Method
cpg	858.45	J/mol×K	1042.84	Joback Method
dvisc	0.0005160	Pa×s	518.32	Joback Method

dvisc	0.0003094	Pa×s	571.58	Joback Method
dvisc	0.0002025	Pa×s	624.84	Joback Method
dvisc	0.0001416	Pa×s	678.10	Joback Method
dvisc	0.0001043	Pa×s	731.37	Joback Method
dvisc	0.0000801	Pa×s	784.63	Joback Method
dvisc	0.0000636	Pa×s	837.89	Joback Method

Sources

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=U353616&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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