Succinic acid, 3,5-dichlorophenyl isobutyl ester

Inchi: InChI=1S/C14H16Cl2O4/c1-9(2)8-19-13(17)3-4-14(18)20-12-6-10(15)5-11(16)7-12/h5-7,

InchiKey: KJLLZEAVRZFQCY-UHFFFAOYSA-N

Formula: C14H16Cl2O4

SMILES: CC(C)COC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1

Mol. weight [g/mol]: 319.18

Physical Properties

Property code	Value	Unit	Source
gf	-333.99	kJ/mol	Joback Method
hf	-645.06	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	77.05	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.878		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2106.00		NIST Webbook
tb	783.36	K	Joback Method
tc	1000.10	K	Joback Method
tf	488.16	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.53	J/mol×K	783.36	Joback Method
cpg	601.85	J/mol×K	819.48	Joback Method
cpg	613.20	J/mol×K	855.61	Joback Method
cpg	623.60	J/mol×K	891.73	Joback Method
cpg	633.05	J/mol×K	927.85	Joback Method
cpg	641.56	J/mol×K	963.98	Joback Method
cpg	649.13	J/mol×K	1000.10	Joback Method
dvisc	0.0006953	Pa×s	488.16	Joback Method
dvisc	0.0004209	Pa×s	537.36	Joback Method

dvisc	0.0002771	Pa×s	586.56	Joback Method
dvisc	0.0001947	Pa×s	635.76	Joback Method
dvisc	0.0001439	Pa×s	684.96	Joback Method
dvisc	0.0001107	Pa×s	734.16	Joback Method
dvisc	0.0000881	Pa×s	783.36	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=U349720&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