Succinic acid, isobutyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C14H15Cl3O4/c1-8(2)7-20-11(18)5-6-12(19)21-14-10(16)4-3-9(15)13(14)17/h3

InchiKey: DLAVXKZVZGRPFU-UHFFFAOYSA-N

Formula: C14H15Cl3O4

SMILES: CC(C)COC(=O)CCC(=O)Oc1c(Cl)ccc(Cl)c1Cl

Mol. weight [g/mol]: 353.62

Physical Properties

Property code	Value	Unit	Source
gf	-355.55	kJ/mol	Joback Method
hf	-672.27	kJ/mol	Joback Method
hfus	39.53	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.532		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	825.77	K	Joback Method
tc	1046.49	K	Joback Method
tf	530.60	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.41	J/mol×K	825.77	Joback Method
cpg	656.15	J/mol×K	1009.70	Joback Method
cpg	648.94	J/mol×K	972.92	Joback Method
cpg	640.77	J/mol×K	936.13	Joback Method
cpg	631.62	J/mol×K	899.34	Joback Method
cpg	621.51	J/mol×K	862.56	Joback Method
cpg	662.39	J/mol×K	1046.49	Joback Method
dvisc	0.0000775	Pa×s	825.77	Joback Method

dvisc	0.0000961	Pa×s	776.58	Joback Method
dvisc	0.0001226	Pa×s	727.38	Joback Method
dvisc	0.0001620	Pa×s	678.18	Joback Method
dvisc	0.0002236	Pa×s	628.99	Joback Method
dvisc	0.0003261	Pa×s	579.80	Joback Method
dvisc	0.0005101	Pa×s	530.60	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=U349703&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