Succinic acid, 2,3-dichlorophenyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-10(16(2,3)4)21-13(19)8-9-14(20)22-12-7-5-6-11(17)15(12)18

InchiKey: FMDYACFBWSQBAM-UHFFFAOYSA-N

Formula: C16H20Cl2O4

SMILES: CC(OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl)C(C)(C)C

Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-314.31	kJ/mol	Joback Method
hf	-695.09	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	80.21	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.657		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook
tb	825.89	K	Joback Method
tc	1046.91	K	Joback Method
tf	513.12	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.00	J/mol×K	825.89	Joback Method
cpg	714.12	J/mol×K	862.73	Joback Method
cpg	726.16	J/mol×K	899.56	Joback Method
cpg	737.15	J/mol×K	936.40	Joback Method
cpg	747.13	J/mol×K	973.24	Joback Method
cpg	756.13	J/mol×K	1010.07	Joback Method
cpg	764.19	J/mol×K	1046.91	Joback Method
dvisc	0.0005262	Pa×s	513.12	Joback Method

dvisc	0.0003011	Pa×s	565.25	Joback Method
dvisc	0.0001894	Pa×s	617.38	Joback Method
dvisc	0.0001280	Pa×s	669.50	Joback Method
dvisc	0.0000916	Pa×s	721.63	Joback Method
dvisc	0.0000685	Pa×s	773.76	Joback Method
dvisc	0.0000532	Pa×s	825.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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