Succinic acid, 2,3-dichlorophenyl 4-methylpent-2-yl ester

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

InchiKey: YAGUWRKVPGMTAH-UHFFFAOYSA-N

Formula: C16H20Cl2O4

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

Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-319.59	kJ/mol	Joback Method
hf	-691.62	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.657		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	828.68	K	Joback Method
tc	1044.31	K	Joback Method
tf	495.70	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.03	J/mol×K	828.68	Joback Method
cpg	754.80	J/mol×K	1008.37	Joback Method
cpg	745.95	J/mol×K	972.43	Joback Method
cpg	736.06	J/mol×K	936.49	Joback Method
cpg	725.12	J/mol×K	900.56	Joback Method
cpg	713.11	J/mol×K	864.62	Joback Method
cpg	762.63	J/mol×K	1044.31	Joback Method
dvisc	0.0000613	Pa×s	828.68	Joback Method

dvisc	0.0000789	Pa×s	773.18	Joback Method
dvisc	0.0001054	Pa×s	717.69	Joback Method
dvisc	0.0001480	Pa×s	662.19	Joback Method
dvisc	0.0002210	Pa×s	606.69	Joback Method
dvisc	0.0003577	Pa×s	551.20	Joback Method
dvisc	0.0006451	Pa×s	495.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390435&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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