Succinic acid, 2,3-dichlorophenyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C18H20Cl2O4/c1-12-5-2-3-6-13(12)11-23-16(21)9-10-17(22)24-15-8-4-7-14(19

InchiKey: CMNRSCTZNRFRDX-UHFFFAOYSA-N

Formula: C18H20Cl2O4

SMILES: CC1=C(COC(=O)CCC(=O)Oc2cccc(Cl)c2Cl)CCCC1

Mol. weight [g/mol]: 371.25

Physical Properties

Property code	Value	Unit	Source
gf	-255.01	kJ/mol	Joback Method
hf	-612.84	kJ/mol	Joback Method
hfus	40.81	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.113		Crippen Method
mcvol	264.920	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	908.66	K	Joback Method
tc	1141.85	K	Joback Method
tf	585.66	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.75	J/mol×K	908.66	Joback Method
cpg	781.25	J/mol×K	947.52	Joback Method
cpg	792.39	J/mol×K	986.39	Joback Method
cpg	802.19	J/mol×K	1025.25	Joback Method
cpg	810.68	J/mol×K	1064.12	Joback Method
cpg	817.88	J/mol×K	1102.98	Joback Method
cpg	823.80	J/mol×K	1141.85	Joback Method
dvisc	0.0003376	Pa×s	585.66	Joback Method

dvisc	0.0002134	Pa×s	639.49	Joback Method
dvisc	0.0001449	Pa×s	693.33	Joback Method
dvisc	0.0001040	Pa×s	747.16	Joback Method
dvisc	0.0000781	Pa×s	800.99	Joback Method
dvisc	0.0000608	Pa×s	854.83	Joback Method
dvisc	0.0000487	Pa×s	908.66	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=U391423&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