Succinic acid, 2,3-dichlorophenyl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C17H20Cl2O4/c1-11-5-7-12(8-6-11)22-15(20)9-10-16(21)23-14-4-2-3-13(18)17

InchiKey: LAAJLVGJKSMGKB-UHFFFAOYSA-N

Formula: C17H20Cl2O4

SMILES: CC1CCC(OC(=O)CCC(=O)Oc2cccc(Cl)c2Cl)CC1

Mol. weight [g/mol]: 359.24

Physical Properties

Property code	Value	Unit	Source
gf	-289.55	kJ/mol	Joback Method
hf	-667.72	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	84.24	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.801		Crippen Method
mcvol	255.130	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	867.32	K	Joback Method
tc	1099.89	K	Joback Method
tf	540.11	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.80	J/mol×K	867.32	Joback Method
cpg	808.73	J/mol×K	1061.13	Joback Method
cpg	800.50	J/mol×K	1022.37	Joback Method
cpg	790.80	J/mol×K	983.61	Joback Method
cpg	779.63	J/mol×K	944.84	Joback Method
cpg	766.97	J/mol×K	906.08	Joback Method
cpg	815.51	J/mol×K	1099.89	Joback Method
dvisc	0.0000853	Pa×s	867.32	Joback Method

dvisc	0.0001059	Pa×s	812.78	Joback Method
dvisc	0.0001357	Pa×s	758.25	Joback Method
dvisc	0.0001806	Pa×s	703.71	Joback Method
dvisc	0.0002522	Pa×s	649.18	Joback Method
dvisc	0.0003745	Pa×s	594.64	Joback Method
dvisc	0.0006022	Pa×s	540.11	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=U390073&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