Succinic acid, 3-chlorophenyl 2-methoxyphenyl ester

Inchi: InChI=1S/C17H15ClO5/c1-21-14-7-2-3-8-15(14)23-17(20)10-9-16(19)22-13-6-4-5-12(18)

InchiKey: IAMLQXIVGOUULN-UHFFFAOYSA-N

Formula: C17H15ClO5

SMILES: COc1ccccc1OC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 334.75

Physical Properties

Property code	Value	Unit	Source
gf	-286.95	kJ/mol	Joback Method
hf	-581.65	kJ/mol	Joback Method
hfus	38.05	kJ/mol	Joback Method
hvap	84.42	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.640		Crippen Method
mcvol	235.860	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	2579.00		NIST Webbook
rinpol	2579.00		NIST Webbook
tb	864.11	K	Joback Method
tc	1097.14	K	Joback Method
tf	555.70	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.88	J/mol×K	864.11	Joback Method
cpg	671.54	J/mol×K	902.95	Joback Method
cpg	681.91	J/mol×K	941.79	Joback Method
cpg	691.00	J/mol×K	980.63	Joback Method
cpg	698.81	J/mol×K	1019.47	Joback Method
cpg	705.34	J/mol×K	1058.31	Joback Method
cpg	710.61	J/mol×K	1097.14	Joback Method
dvisc	0.0003644	Pa×s	555.70	Joback Method

dvisc	0.0002341	Pa×s	607.10	Joback Method
dvisc	0.0001611	Pa×s	658.50	Joback Method
dvisc	0.0001171	Pa×s	709.90	Joback Method
dvisc	0.0000888	Pa×s	761.31	Joback Method
dvisc	0.0000698	Pa×s	812.71	Joback Method
dvisc	0.0000564	Pa×s	864.11	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=U389713&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

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