Succinic acid, 3-chlorophenyl 4-methoxybenzyl ester

Inchi: InChI=1S/C18H17ClO5/c1-22-15-7-5-13(6-8-15)12-23-17(20)9-10-18(21)24-16-4-2-3-14(

InchiKey: BGOBLKRUBZZPLL-UHFFFAOYSA-N

Formula: C18H17ClO5

SMILES: COc1ccc(COC(=O)CCC(=O)Oc2cccc(Cl)c2)cc1

Mol. weight [g/mol]: 348.78

Physical Properties

Property code	Value	Unit	Source
gf	-278.53	kJ/mol	Joback Method
hf	-602.29	kJ/mol	Joback Method
hfus	40.64	kJ/mol	Joback Method
hvap	86.65	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.778		Crippen Method
mcvol	249.950	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	2776.00		NIST Webbook
rinpol	2776.00		NIST Webbook
tb	886.99	K	Joback Method
tc	1117.53	K	Joback Method
tf	566.97	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.76	J/mol×K	886.99	Joback Method
cpg	727.55	J/mol×K	925.41	Joback Method
cpg	738.00	J/mol×K	963.84	Joback Method
cpg	747.15	J/mol×K	1002.26	Joback Method
cpg	754.98	J/mol×K	1040.69	Joback Method
cpg	761.53	J/mol×K	1079.11	Joback Method
cpg	766.80	J/mol×K	1117.53	Joback Method
dvisc	0.0003311	Pa×s	566.97	Joback Method

dvisc	0.0002101	Pa×s	620.31	Joback Method
dvisc	0.0001433	Pa×s	673.64	Joback Method
dvisc	0.0001033	Pa×s	726.98	Joback Method
dvisc	0.0000779	Pa×s	780.32	Joback Method
dvisc	0.0000610	Pa×s	833.65	Joback Method
dvisc	0.0000491	Pa×s	886.99	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=U389693&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