Succinic acid, 4-chloro-3-methylphenyl 2-methoxyphenyl ester

Inchi: InChI=1S/C18H17ClO5/c1-12-11-13(7-8-14(12)19)23-17(20)9-10-18(21)24-16-6-4-3-5-15

InchiKey: LANBFZORMQJGPL-UHFFFAOYSA-N

Formula: C18H17ClO5

SMILES: COc1ccccc1OC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 348.78

Physical Properties

Property code	Value	Unit	Source
gf	-288.16	kJ/mol	Joback Method
hf	-613.76	kJ/mol	Joback Method
hfus	40.25	kJ/mol	Joback Method
hvap	87.31	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.948		Crippen Method
mcvol	249.950	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook
tb	891.97	K	Joback Method
tc	1123.25	K	Joback Method
tf	579.49	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.28	J/mol×K	891.97	Joback Method
cpg	725.95	J/mol×K	930.52	Joback Method
cpg	736.28	J/mol×K	969.06	Joback Method
cpg	745.27	J/mol×K	1007.61	Joback Method
cpg	752.93	J/mol×K	1046.16	Joback Method
cpg	759.26	J/mol×K	1084.71	Joback Method
cpg	764.25	J/mol×K	1123.25	Joback Method
dvisc	0.0002970	Pa×s	579.49	Joback Method

dvisc	0.0001952	Pa×s	631.57	Joback Method
dvisc	0.0001368	Pa×s	683.65	Joback Method
dvisc	0.0001008	Pa×s	735.73	Joback Method
dvisc	0.0000774	Pa×s	787.81	Joback Method
dvisc	0.0000613	Pa×s	839.89	Joback Method
dvisc	0.0000500	Pa×s	891.97	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=U389715&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