

Succinic acid, 3-chlorophenyl 2-methoxy-5-methylphenyl ester

Inchi:	InChI=1S/C18H17ClO5/c1-12-6-7-15(22-2)16(10-12)24-18(21)9-8-17(20)23-14-5-3-4-13
InchiKey:	AEPOVYZFEKJQPT-UHFFFAOYSA-N
Formula:	C18H17ClO5
SMILES:	COc1ccc(C)cc1OC(=O)CCC(=O)Oc1cccc(Cl)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	2678.00		NIST Webbook
rinpol	2678.00		NIST Webbook
tb	891.97	K	Joback Method
tc	1123.25	K	Joback Method
tf	579.49	K	Joback Method
vc	0.943	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001952	Paxs	631.57	Joback Method
dvisc	0.0001368	Paxs	683.65	Joback Method
dvisc	0.0001008	Paxs	735.73	Joback Method
dvisc	0.0000774	Paxs	787.81	Joback Method
dvisc	0.0000613	Paxs	839.89	Joback Method
dvisc	0.0000500	Paxs	891.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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