

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

Inchi:	InChI=1S/C19H19ClO4/c1-12-5-4-6-17(14(12)3)24-19(22)10-9-18(21)23-15-7-8-16(20)1
InchiKey:	KHFOAWJTIQLLAI-UHFFFAOYSA-N
Formula:	C19H19ClO4
SMILES:	<chem>Cc1cc(OC(=O)CCC(=O)Oc2cccc(C)c2C)ccc1Cl</chem>
Mol. weight [g/mol]:	346.81

Physical Properties

Property code	Value	Unit	Source
gf	-184.37	kJ/mol	Joback Method
hf	-513.65	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.556		Crippen Method
mvol	258.170	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2775.00		NIST Webbook
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tb	897.41	K	Joback Method
tc	1128.66	K	Joback Method
tf	581.05	K	Joback Method
vc	0.981	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.49	J/molxK	897.41	Joback Method
cpg	792.81	J/molxK	1090.12	Joback Method
cpg	785.44	J/molxK	1051.58	Joback Method
cpg	776.84	J/molxK	1013.04	Joback Method
cpg	766.99	J/molxK	974.49	Joback Method
cpg	755.88	J/molxK	935.95	Joback Method
cpg	798.96	J/molxK	1128.66	Joback Method
dvisc	0.0000591	Paxs	897.41	Joback Method

dvisc	0.0000721	Paxs	844.68	Joback Method
dvisc	0.0000904	Paxs	791.96	Joback Method
dvisc	0.0001170	Paxs	739.23	Joback Method
dvisc	0.0001577	Paxs	686.50	Joback Method
dvisc	0.0002233	Paxs	633.78	Joback Method
dvisc	0.0003367	Paxs	581.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390028&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

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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