

Succinic acid, 4-chloro-3-methylphenyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi:	InChI=1S/C19H23ClO4/c1-13-5-3-4-6-15(13)12-23-18(21)9-10-19(22)24-16-7-8-17(20)1
InchiKey:	KBZWIHUVYXQDEE-UHFFFAOYSA-N
Formula:	C19H23ClO4
SMILES:	CC1=C(COC(=O)CCC(=O)Oc2ccc(Cl)c(C)c2)CCCC1
Mol. weight [g/mol]:	350.84

Physical Properties

Property code	Value	Unit	Source
gf	-234.66	kJ/mol	Joback Method
hf	-617.74	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	86.54	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.768		Crippen Method
mcvol	266.770	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
tb	894.11	K	Joback Method
tc	1122.11	K	Joback Method
tf	567.01	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.69	J/molxK	894.11	Joback Method
cpg	860.12	J/molxK	1084.11	Joback Method
cpg	851.51	J/molxK	1046.11	Joback Method
cpg	841.58	J/molxK	1008.11	Joback Method
cpg	830.32	J/molxK	970.11	Joback Method
cpg	817.69	J/molxK	932.11	Joback Method
cpg	867.43	J/molxK	1122.11	Joback Method
dvisc	0.0000492	Paxs	894.11	Joback Method
dvisc	0.0000616	Paxs	839.59	Joback Method
dvisc	0.0000797	Paxs	785.08	Joback Method

dvisc	0.0001072	Paxs	730.56	Joback Method
dvisc	0.0001511	Paxs	676.04	Joback Method
dvisc	0.0002263	Paxs	621.53	Joback Method
dvisc	0.0003662	Paxs	567.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391422&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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