Succinic acid, 4-chloro-3-methylphenyl cis-4-methylcyclohexyl ester

Inchi: InChI=1S/C18H23ClO4/c1-12-3-5-14(6-4-12)22-17(20)9-10-18(21)23-15-7-8-16(19)13(2)

InchiKey: YJONPWCLHGBIOL-UHFFFAOYSA-N

Formula: C18H23ClO4

SMILES: Cc1cc(OC(=O)CCC(=O)OC2CCC(C)CC2)ccc1Cl

Mol. weight [g/mol]: 338.83

Physical Properties

Property code	Value	Unit	Source
gf	-269.20	kJ/mol	Joback Method
hf	-672.62	kJ/mol	Joback Method
hfus	38.32	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.456		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook
tb	852.77	K	Joback Method
tc	1079.80	K	Joback Method
tf	521.46	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.60	J/mol×K	852.77	Joback Method
cpg	801.34	J/mol×K	890.61	Joback Method
cpg	815.58	J/mol×K	928.45	Joback Method
cpg	828.31	J/mol×K	966.29	Joback Method
cpg	839.56	J/mol×K	1004.13	Joback Method
cpg	849.33	J/mol×K	1041.96	Joback Method
cpg	857.65	J/mol×K	1079.80	Joback Method
dvisc	0.0006484	Pa×s	521.46	Joback Method

dvisc	0.0003934	Pa×s	576.68	Joback Method
dvisc	0.0002605	Pa×s	631.90	Joback Method
dvisc	0.0001843	Pa×s	687.12	Joback Method
dvisc	0.0001373	Pa×s	742.33	Joback Method
dvisc	0.0001065	Pa×s	797.55	Joback Method
dvisc	0.0000854	Pa×s	852.77	Joback Method

Sources

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=U390060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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