Succinic acid, 2-chloro-5-methylphenyl isohexyl ester

Inchi: InChI=1S/C17H23ClO4/c1-12(2)5-4-10-21-16(19)8-9-17(20)22-15-11-13(3)6-7-14(15)18/

InchiKey: ZFWJOZYDQHLGDD-UHFFFAOYSA-N

Formula: C17H23ClO4

SMILES: Cc1ccc(Cl)c(OC(=O)CCC(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 326.81

Physical Properties

Property code	Value	Unit	Source
gf	-296.80	kJ/mol	Joback Method
hf	-691.24	kJ/mol	Joback Method
hfus	39.30	kJ/mol	Joback Method
hvap	79.34	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.313		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook
tb	814.57	K	Joback Method
tc	1022.39	K	Joback Method
tf	492.05	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.92	J/mol×K	814.57	Joback Method
cpg	745.28	J/mol×K	849.21	Joback Method
cpg	758.58	J/mol×K	883.84	Joback Method
cpg	770.83	J/mol×K	918.48	Joback Method
cpg	782.05	J/mol×K	953.12	Joback Method
cpg	792.25	J/mol×K	987.76	Joback Method
cpg	801.44	J/mol×K	1022.39	Joback Method
dvisc	0.0006311	Pa×s	492.05	Joback Method

dvisc	0.0003612	Pa×s	545.80	Joback Method
dvisc	0.0002285	Pa×s	599.56	Joback Method
dvisc	0.0001559	Pa×s	653.31	Joback Method
dvisc	0.0001127	Pa×s	707.06	Joback Method
dvisc	0.0000853	Pa×s	760.82	Joback Method
dvisc	0.0000670	Pa×s	814.57	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=U353328&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

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