Succinic acid, 4-chloro-3-methylphenyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C18H25ClO4/c1-11(2)18(12(3)4)23-17(21)9-8-16(20)22-14-6-7-15(19)13(5)10-

InchiKey: GSUDTPLVGFTSNF-UHFFFAOYSA-N

Formula: C18H25ClO4

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

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-293.26	kJ/mol	Joback Method
hf	-722.44	kJ/mol	Joback Method
hfus	34.84	kJ/mol	Joback Method
hvap	80.80	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.558		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	836.57	K	Joback Method
tc	1048.43	K	Joback Method
tf	473.32	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.10	J/mol×K	836.57	Joback Method
cpg	803.99	J/mol×K	871.88	Joback Method
cpg	817.70	J/mol×K	907.19	Joback Method
cpg	830.26	J/mol×K	942.50	Joback Method
cpg	841.68	J/mol×K	977.81	Joback Method
cpg	851.98	J/mol×K	1013.12	Joback Method
cpg	861.16	J/mol×K	1048.43	Joback Method
dvisc	0.0007391	Pa×s	473.32	Joback Method

dvisc	0.0003639	Pa×s	533.86	Joback Method
dvisc	0.0002070	Pa×s	594.40	Joback Method
dvisc	0.0001307	Pa×s	654.94	Joback Method
dvisc	0.0000892	Pa×s	715.49	Joback Method
dvisc	0.0000646	Pa×s	776.03	Joback Method
dvisc	0.0000490	Pa×s	836.57	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=U390511&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