Succinic acid, cyclohexylmethyl 2-chloro-4-methylphenyl ester

Inchi: InChI=1S/C18H23ClO4/c1-13-7-8-16(15(19)11-13)23-18(21)10-9-17(20)22-12-14-5-3-2-4

InchiKey: DOEDUUIFKHWHLK-UHFFFAOYSA-N

Formula: C18H23ClO4

SMILES: Cc1ccc(OC(=O)CCC(=O)OCC2CCCCC2)c(Cl)c1

Mol. weight [g/mol]: 338.83

Physical Properties

Property code	Value	Unit	Source
gf	-261.49	kJ/mol	Joback Method
hf	-652.28	kJ/mol	Joback Method
hfus	37.24	kJ/mol	Joback Method
hvap	82.39	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.458		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	857.44	K	Joback Method
tc	1084.55	K	Joback Method
tf	525.70	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.43	J/mol×K	857.44	Joback Method
cpg	796.79	J/mol×K	895.29	Joback Method
cpg	810.68	J/mol×K	933.14	Joback Method
cpg	823.15	J/mol×K	971.00	Joback Method
cpg	834.20	J/mol×K	1008.85	Joback Method
cpg	843.87	J/mol×K	1046.70	Joback Method
cpg	852.18	J/mol×K	1084.55	Joback Method
dvisc	0.0005867	Pa×s	525.70	Joback Method

dvisc	0.0003428	Pa×s	580.99	Joback Method
dvisc	0.0002199	Pa×s	636.28	Joback Method
dvisc	0.0001514	Pa×s	691.57	Joback Method
dvisc	0.0001102	Pa×s	746.86	Joback Method
dvisc	0.0000838	Pa×s	802.15	Joback Method
dvisc	0.0000660	Pa×s	857.44	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=U390219&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