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

Inchi: InChI=1S/C18H23ClO5/c1-22-16-11-14(19)7-8-15(16)24-18(21)10-9-17(20)23-12-13-5-3

InchiKey: YIHMJNJJADKHRM-UHFFFAOYSA-N

Formula: C18H23ClO5

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 354.82

Physical Properties

Property code	Value	Unit	Source
gf	-366.49	kJ/mol	Joback Method
hf	-784.50	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	84.80	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.158		Crippen Method
mcvol	262.850	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	879.86	K	Joback Method
tc	1105.70	K	Joback Method
tf	547.93	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.20	J/mol×K	879.86	Joback Method
cpg	823.74	J/mol×K	917.50	Joback Method
cpg	836.75	J/mol×K	955.14	Joback Method
cpg	848.22	J/mol×K	992.78	Joback Method
cpg	858.16	J/mol×K	1030.42	Joback Method
cpg	866.58	J/mol×K	1068.06	Joback Method
cpg	873.48	J/mol×K	1105.70	Joback Method
dvisc	0.0004150	Pa×s	547.93	Joback Method

dvisc	0.0002474	Pa×s	603.25	Joback Method
dvisc	0.0001609	Pa×s	658.57	Joback Method
dvisc	0.0001119	Pa×s	713.89	Joback Method
dvisc	0.0000819	Pa×s	769.22	Joback Method
dvisc	0.0000626	Pa×s	824.54	Joback Method
dvisc	0.0000494	Pa×s	879.86	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=U390940&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