Succinic acid, 2-methoxy-4-chlorobenzyl undecyl ester

Inchi: InChI=1S/C23H35ClO5/c1-3-4-5-6-7-8-9-10-11-16-28-22(25)14-15-23(26)29-18-19-12-13

InchiKey: FEDYPDWESUFSKY-UHFFFAOYSA-N

Formula: C23H35ClO5

SMILES: CCCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 426.97

Physical Properties

Property code	Value	Unit	Source
gf	-348.84	kJ/mol	Joback Method
hf	-942.02	kJ/mol	Joback Method
hfus	59.55	kJ/mol	Joback Method
hvap	95.50	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.246		Crippen Method
mcvol	344.160	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	3023.00		NIST Webbook
rinpol	3023.00		NIST Webbook
tb	974.71	K	Joback Method
tc	1193.34	K	Joback Method
tf	596.90	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.70	J/mol×K	974.71	Joback Method
cpg	1171.42	J/mol×K	1156.91	Joback Method
cpg	1162.67	J/mol×K	1120.47	Joback Method
cpg	1152.44	J/mol×K	1084.03	Joback Method
cpg	1140.72	J/mol×K	1047.59	Joback Method
cpg	1127.48	J/mol×K	1011.15	Joback Method
cpg	1178.70	J/mol×K	1193.34	Joback Method
dvisc	0.0000229	Pa×s	974.71	Joback Method

dvisc	0.0000292	Pa×s	911.74	Joback Method
dvisc	0.0000386	Pa×s	848.77	Joback Method
dvisc	0.0000534	Pa×s	785.81	Joback Method
dvisc	0.0000781	Pa×s	722.84	Joback Method
dvisc	0.0001230	Pa×s	659.87	Joback Method
dvisc	0.0002130	Pa×s	596.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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