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

Inchi: InChI=1S/C17H23ClO5/c1-3-4-5-10-22-16(19)8-9-17(20)23-12-13-6-7-14(18)11-15(13)21

InchiKey: LUQUNQGQUKZBSE-UHFFFAOYSA-N

Formula: C17H23ClO5

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

Mol. weight [g/mol]: 342.81

Physical Properties

Property code	Value	Unit	Source
gf	-399.36	kJ/mol	Joback Method
hf	-818.18	kJ/mol	Joback Method
hfus	44.01	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.905		Crippen Method
mcvol	259.620	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2434.00		NIST Webbook
rinpol	2434.00		NIST Webbook
tb	837.43	K	Joback Method
tc	1042.91	K	Joback Method
tf	529.28	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.01	J/mol×K	837.43	Joback Method
cpg	771.77	J/mol×K	871.68	Joback Method
cpg	784.43	J/mol×K	905.92	Joback Method
cpg	796.00	J/mol×K	940.17	Joback Method
cpg	806.47	J/mol×K	974.41	Joback Method
cpg	815.84	J/mol×K	1008.66	Joback Method
cpg	824.12	J/mol×K	1042.91	Joback Method
dvisc	0.0004050	Pa×s	529.28	Joback Method

dvisc	0.0002506	Pa×s	580.64	Joback Method
dvisc	0.0001677	Pa×s	632.00	Joback Method
dvisc	0.0001192	Pa×s	683.36	Joback Method
dvisc	0.0000888	Pa×s	734.71	Joback Method
dvisc	0.0000688	Pa×s	786.07	Joback Method
dvisc	0.0000550	Pa×s	837.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380849&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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