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

Inchi: InChI=1S/C22H33ClO5/c1-3-4-5-6-7-8-9-10-15-27-21(24)13-14-22(25)28-17-18-11-12-19
InchiKey: TYGKXTJGRNYOAS-UHFFFAOYSA-N
Formula: C22H33ClO5
SMILES: CCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(Cl)cc1OC
Mol. weight [g/mol]: 412.95

Physical Properties

Property code	Value	Unit	Source
gf	-357.26	kJ/mol	Joback Method
hf	-921.38	kJ/mol	Joback Method
hfus	56.96	kJ/mol	Joback Method
hvap	93.27	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.856		Crippen Method
mcvol	330.070	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2933.00		NIST Webbook
rinpol	2933.00		NIST Webbook
tb	951.83	K	Joback Method
tc	1166.07	K	Joback Method
tf	585.63	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1052.14	J/mol×K	951.83	Joback Method
cpg	1066.77	J/mol×K	987.54	Joback Method
cpg	1079.95	J/mol×K	1023.24	Joback Method
cpg	1091.72	J/mol×K	1058.95	Joback Method
cpg	1102.07	J/mol×K	1094.66	Joback Method
cpg	1111.04	J/mol×K	1130.36	Joback Method
cpg	1118.62	J/mol×K	1166.07	Joback Method
dvisc	0.0002391	Pa×s	585.63	Joback Method

dvisc	0.0001395	Pa×s	646.66	Joback Method
dvisc	0.0000893	Pa×s	707.70	Joback Method
dvisc	0.0000614	Pa×s	768.73	Joback Method
dvisc	0.0000446	Pa×s	829.76	Joback Method
dvisc	0.0000338	Pa×s	890.80	Joback Method
dvisc	0.0000266	Pa×s	951.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380854&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

Latest version available from:
https://www.chemeo.com/cid/95-973-7/Succinic-acid-decyl-2-methoxy-4-chlorobenzyl-ester.pdf
Generated by Cheméo on 2024-10-12 09:44:53.773562973 +0000 UTC m=+3307156.410532222.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.