Succinic acid, 8-chlorooctyl 4-methoxybenzyl ester

Inchi: InChI=1S/C20H29ClO5/c1-24-18-10-8-17(9-11-18)16-26-20(23)13-12-19(22)25-15-7-5-3

InchiKey: VFRPABTUMGHZMC-UHFFFAOYSA-N

Formula: C20H29ClO5

SMILES: COc1ccc(COC(=O)CCC(=O)OCCCCCCCCCCl)cc1

Mol. weight [g/mol]: 384.89

Physical Properties

Property code	Value	Unit	Source
gf	-364.47	kJ/mol	Joback Method
hf	-868.63	kJ/mol	Joback Method
hfus	52.17	kJ/mol	Joback Method
hvap	88.16	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.641		Crippen Method
mcvol	301.890	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
tb	901.09	K	Joback Method
tc	1108.44	K	Joback Method
tf	550.57	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.48	J/mol×K	901.09	Joback Method
cpg	947.89	J/mol×K	935.65	Joback Method
cpg	961.05	J/mol×K	970.21	Joback Method
cpg	972.96	J/mol×K	1004.76	Joback Method
cpg	983.64	J/mol×K	1039.32	Joback Method
cpg	993.10	J/mol×K	1073.88	Joback Method
cpg	1001.35	J/mol×K	1108.44	Joback Method
dvisc	0.0003387	Pa×s	550.57	Joback Method

dvisc	0.0001938	Pa×s	608.99	Joback Method
dvisc	0.0001222	Pa×s	667.41	Joback Method
dvisc	0.0000830	Pa×s	725.83	Joback Method
dvisc	0.0000598	Pa×s	784.25	Joback Method
dvisc	0.0000450	Pa×s	842.67	Joback Method
dvisc	0.0000352	Pa×s	901.09	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=U389696&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