Sebacic acid, ethyl 2-methoxy-4-chlorobenzyl ester

Inchi: InChI=1S/C20H29ClO5/c1-3-25-19(22)10-8-6-4-5-7-9-11-20(23)26-15-16-12-13-17(21)14

InchiKey: MCLGQZPFIGZLNR-UHFFFAOYSA-N

Formula: C20H29ClO5

SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 384.89

Physical Properties

Property code	Value	Unit	Source
gf	-374.10	kJ/mol	Joback Method
hf	-880.10	kJ/mol	Joback Method
hfus	51.78	kJ/mol	Joback Method
hvap	88.82	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.076		Crippen Method
mcvol	301.890	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	906.07	K	Joback Method
tc	1114.34	K	Joback Method
tf	563.09	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.56	J/mol×K	906.07	Joback Method
cpg	946.87	J/mol×K	940.78	Joback Method
cpg	959.91	J/mol×K	975.49	Joback Method
cpg	971.68	J/mol×K	1010.21	Joback Method
cpg	982.19	J/mol×K	1044.92	Joback Method
cpg	991.44	J/mol×K	1079.63	Joback Method
cpg	999.45	J/mol×K	1114.34	Joback Method
dvisc	0.0002985	Pa×s	563.09	Joback Method

dvisc	0.0001781	Pa×s	620.25	Joback Method
dvisc	0.0001160	Pa×s	677.42	Joback Method
dvisc	0.0000807	Pa×s	734.58	Joback Method
dvisc	0.0000592	Pa×s	791.74	Joback Method
dvisc	0.0000453	Pa×s	848.91	Joback Method
dvisc	0.0000358	Pa×s	906.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380634&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