Sebacic acid, di(2-methoxy-4-chlorobenzyl) ester

Inchi: InChI=1S/C26H32Cl2O6/c1-31-23-15-21(27)13-11-19(23)17-33-25(29)9-7-5-3-4-6-8-10-2

InchiKey: ZSQLJMMLGNWAAA-UHFFFAOYSA-N

Formula: C26H32Cl2O6

SMILES: COc1cc(Cl)ccc1COC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 511.44

Physical Properties

Property code	Value	Unit	Source
gf	-347.36	kJ/mol	Joback Method
hf	-938.31	kJ/mol	Joback Method
hfus	65.97	kJ/mol	Joback Method
hvap	112.57	kJ/mol	Joback Method
log10ws	-8.40		Crippen Method
logp	6.918		Crippen Method
mcvol	380.780	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	3610.00		NIST Webbook
rinpol	3610.00		NIST Webbook
tb	1139.84	K	Joback Method
tc	1397.45	K	Joback Method
tf	734.32	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.25	J/mol×K	1139.84	Joback Method
cpg	1235.91	J/mol×K	1354.52	Joback Method
cpg	1237.61	J/mol×K	1311.58	Joback Method
cpg	1237.01	J/mol×K	1268.65	Joback Method
cpg	1234.10	J/mol×K	1225.71	Joback Method
cpg	1228.85	J/mol×K	1182.78	Joback Method
cpg	1231.91	J/mol×K	1397.45	Joback Method
dvisc	0.0000097	Pa×s	1139.84	Joback Method

dvisc	0.0000120	Pa×s	1072.25	Joback Method
dvisc	0.0000154	Pa×s	1004.67	Joback Method
dvisc	0.0000205	Pa×s	937.08	Joback Method
dvisc	0.0000284	Pa×s	869.49	Joback Method
dvisc	0.0000416	Pa×s	801.91	Joback Method
dvisc	0.0000655	Pa×s	734.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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