Sebacic acid, 2-methoxy-4-chlorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C25H39ClO5/c1-5-12-22(19(2)3)31-25(28)14-11-9-7-6-8-10-13-24(27)30-18-20

InchiKey: CLKSXZLKXSKQEF-UHFFFAOYSA-N

Formula: C25H39ClO5

SMILES: CCCC(OC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)cc1OC)C(C)C

Mol. weight [g/mol]: 455.03

Physical Properties

Property code	Value	Unit	Source
gf	-336.88	kJ/mol	Joback Method
hf	-993.86	kJ/mol	Joback Method
hfus	57.68	kJ/mol	Joback Method
hvap	99.17	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.881		Crippen Method
mcvol	372.340	ml/mol	McGowan Method
pc	939.22	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	1019.59	K	Joback Method
tc	1248.82	K	Joback Method
tf	589.44	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1235.70	J/mol×K	1019.59	Joback Method
cpg	1250.56	J/mol×K	1057.79	Joback Method
cpg	1263.64	J/mol×K	1096.00	Joback Method
cpg	1274.96	J/mol×K	1134.20	Joback Method
cpg	1284.55	J/mol×K	1172.41	Joback Method
cpg	1292.44	J/mol×K	1210.61	Joback Method
cpg	1298.66	J/mol×K	1248.82	Joback Method
dvisc	0.0001963	Pa×s	589.44	Joback Method

dvisc	0.0000994	Pa×s	661.13	Joback Method
dvisc	0.0000575	Pa×s	732.82	Joback Method
dvisc	0.0000366	Pa×s	804.51	Joback Method
dvisc	0.0000251	Pa×s	876.21	Joback Method
dvisc	0.0000183	Pa×s	947.90	Joback Method
dvisc	0.0000139	Pa×s	1019.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380635&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