Sebacic acid, 2-methoxybenzyl pentyl ester

Inchi: InChI=1S/C23H36O5/c1-3-4-13-18-27-22(24)16-9-7-5-6-8-10-17-23(25)28-19-20-14-11-1
InchiKey: OAAGTHDZOBTNLQ-UHFFFAOYSA-N
Formula: C23H36O5
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1OC
Mol. weight [g/mol]: 392.53

Physical Properties

Property code	Value	Unit	Source
gf	-327.28	kJ/mol	Joback Method
hf	-914.81	kJ/mol	Joback Method
hfus	55.74	kJ/mol	Joback Method
hvap	90.45	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.593		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	932.30	K	Joback Method
tc	1142.00	K	Joback Method
tf	554.46	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.84	J/mol×K	932.30	Joback Method
cpg	1154.64	J/mol×K	1107.05	Joback Method
cpg	1144.07	J/mol×K	1072.10	Joback Method
cpg	1132.12	J/mol×K	1037.15	Joback Method
cpg	1118.78	J/mol×K	1002.20	Joback Method
cpg	1104.03	J/mol×K	967.25	Joback Method
cpg	1163.87	J/mol×K	1142.00	Joback Method
dvisc	0.0000265	Pa×s	932.30	Joback Method

dvisc	0.0000343	Pa×s	869.33	Joback Method
dvisc	0.0000462	Pa×s	806.35	Joback Method
dvisc	0.0000654	Pa×s	743.38	Joback Method
dvisc	0.0000989	Pa×s	680.41	Joback Method
dvisc	0.0001626	Pa×s	617.43	Joback Method
dvisc	0.0002993	Pa×s	554.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380774&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