Sebacic acid, isohexyl 4-methoxyphenyl ester

Inchi: InChI=1S/C23H36O5/c1-19(2)11-10-18-27-22(24)12-8-6-4-5-7-9-13-23(25)28-21-16-14-2
InchiKey: BIHCQNWOSIRHLC-UHFFFAOYSA-N
Formula: C23H36O5
SMILES: COc1ccc(OC(=O)CCCCCCCCC(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]: 392.53

Physical Properties

Property code	Value	Unit	Source
gf	-329.72	kJ/mol	Joback Method
hf	-920.09	kJ/mol	Joback Method
hfus	52.22	kJ/mol	Joback Method
hvap	90.06	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.701		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	3003.00		NIST Webbook
rinpol	3003.00		NIST Webbook
tb	931.86	K	Joback Method
tc	1141.96	K	Joback Method
tf	539.46	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.27	J/mol×K	931.86	Joback Method
cpg	1104.46	J/mol×K	966.88	Joback Method
cpg	1119.19	J/mol×K	1001.89	Joback Method
cpg	1132.49	J/mol×K	1036.91	Joback Method
cpg	1144.38	J/mol×K	1071.93	Joback Method
cpg	1154.88	J/mol×K	1106.95	Joback Method
cpg	1164.02	J/mol×K	1141.96	Joback Method
dvisc	0.0003316	Pa×s	539.46	Joback Method

dvisc	0.0001693	Pa×s	604.86	Joback Method
dvisc	0.0000985	Pa×s	670.26	Joback Method
dvisc	0.0000631	Pa×s	735.66	Joback Method
dvisc	0.0000435	Pa×s	801.06	Joback Method
dvisc	0.0000317	Pa×s	866.46	Joback Method
dvisc	0.0000242	Pa×s	931.86	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=U354776&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