Sebacic acid, isohexyl 4-methoxy-2-methylbutyl ester

Other names: Sebacic acid, isohexyl 4-methoxy-2-methylphenyl ester
Inchi: InChI=1S/C22H42O5/c1-19(2)12-11-16-26-21(23)13-9-7-5-6-8-10-14-22(24)27-18-20(3)1
InchiKey: DOUKKXLHMOXFNX-UHFFFAOYSA-N
Formula: C22H42O5
SMILES: COCCC(C)COC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 386.57

Physical Properties

Property code	Value	Unit	Source
gf	-443.36	kJ/mol	Joback Method
hf	-1129.79	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.302		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	876.88	K	Joback Method
tc	1073.55	K	Joback Method
tf	474.25	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.01	J/mol×K	876.88	Joback Method
cpg	1143.87	J/mol×K	909.66	Joback Method
cpg	1161.39	J/mol×K	942.44	Joback Method
cpg	1177.58	J/mol×K	975.22	Joback Method
cpg	1192.45	J/mol×K	1008.00	Joback Method
cpg	1206.02	J/mol×K	1040.78	Joback Method
cpg	1218.30	J/mol×K	1073.55	Joback Method

dvisc	0.0006124	Pa×s	474.25	Joback Method
dvisc	0.0002574	Pa×s	541.36	Joback Method
dvisc	0.0001310	Pa×s	608.46	Joback Method
dvisc	0.0000762	Pa×s	675.57	Joback Method
dvisc	0.0000489	Pa×s	742.67	Joback Method
dvisc	0.0000338	Pa×s	809.78	Joback Method
dvisc	0.0000247	Pa×s	876.88	Joback Method

Sources

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=U355325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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