Sebacic acid, isohexyl 3-methylphenyl ester

Inchi: InChI=1S/C23H36O4/c1-19(2)12-11-17-26-22(24)15-8-6-4-5-7-9-16-23(25)27-21-14-10-1
InchiKey: MJHDDBXBGJVAIS-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: Cc1cccc(OC(=O)CCCCCCCCC(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-224.72	kJ/mol	Joback Method
hf	-787.87	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.001		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		NIST Webbook
tb	909.44	K	Joback Method
tc	1116.16	K	Joback Method
tf	517.23	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.53	J/mol×K	909.44	Joback Method
cpg	1075.35	J/mol×K	943.89	Joback Method
cpg	1090.85	J/mol×K	978.35	Joback Method
cpg	1105.07	J/mol×K	1012.80	Joback Method
cpg	1118.04	J/mol×K	1047.26	Joback Method
cpg	1129.80	J/mol×K	1081.71	Joback Method
cpg	1140.38	J/mol×K	1116.16	Joback Method
dvisc	0.0004827	Pa×s	517.23	Joback Method

dvisc	0.0002394	Pa×s	582.60	Joback Method
dvisc	0.0001368	Pa×s	647.97	Joback Method
dvisc	0.0000866	Pa×s	713.34	Joback Method
dvisc	0.0000592	Pa×s	778.70	Joback Method
dvisc	0.0000429	Pa×s	844.07	Joback Method
dvisc	0.0000326	Pa×s	909.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354927&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

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