Sebacic acid, isohexyl oct-3-en-2-yl ester

Inchi: InChI=1S/C24H44O4/c1-5-6-7-12-17-22(4)28-24(26)19-14-11-9-8-10-13-18-23(25)27-20
InchiKey: DEEIJEDMIWYIAI-SFQUDFHCSA-N
Formula: C24H44O4
SMILES: CCCCC=CC(C)OC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-241.30	kJ/mol	Joback Method
hf	-921.63	kJ/mol	Joback Method
hfus	56.65	kJ/mol	Joback Method
hvap	86.51	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.765		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	884.72	kPa	Joback Method
rinpol	2628.00		NIST Webbook
tb	904.38	K	Joback Method
tc	1107.28	K	Joback Method
tf	469.48	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.39	J/mol×K	904.38	Joback Method
cpg	1276.05	J/mol×K	1073.46	Joback Method
cpg	1261.54	J/mol×K	1039.64	Joback Method
cpg	1245.87	J/mol×K	1005.83	Joback Method
cpg	1228.98	J/mol×K	972.01	Joback Method
cpg	1210.84	J/mol×K	938.20	Joback Method
cpg	1289.44	J/mol×K	1107.28	Joback Method
dvisc	0.0000215	Pa×s	904.38	Joback Method
dvisc	0.0000297	Pa×s	831.90	Joback Method

dvisc	0.0000436	Pa×s	759.41	Joback Method
dvisc	0.0000695	Pa×s	686.93	Joback Method
dvisc	0.0001238	Pa×s	614.45	Joback Method
dvisc	0.0002572	Pa×s	541.96	Joback Method
dvisc	0.0006695	Pa×s	469.48	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=U355838&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

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