Sebacic acid, isohexyl trans-3-hexenyl ester

Inchi: InChI=1S/C22H40O4/c1-4-5-6-13-18-25-21(23)16-11-9-7-8-10-12-17-22(24)26-19-14-15
InchiKey: ONRCGOHVOXTDPZ-AATRIKPKSA-N
Formula: C22H40O4
SMILES: CCC=CCCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-255.70	kJ/mol	Joback Method
hf	-875.07	kJ/mol	Joback Method
hfus	54.99	kJ/mol	Joback Method
hvap	82.45	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.986		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	2537.00		NIST Webbook
tb	859.06	K	Joback Method
tc	1052.46	K	Joback Method
tf	461.94	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.29	J/mol×K	859.06	Joback Method
cpg	1148.14	J/mol×K	1020.23	Joback Method
cpg	1133.90	J/mol×K	987.99	Joback Method
cpg	1118.63	J/mol×K	955.76	Joback Method
cpg	1102.30	J/mol×K	923.53	Joback Method
cpg	1084.86	J/mol×K	891.29	Joback Method
cpg	1161.37	J/mol×K	1052.46	Joback Method
dvisc	0.0000317	Pa×s	859.06	Joback Method
dvisc	0.0000430	Pa×s	792.87	Joback Method

dvisc	0.0000617	Pa×s	726.69	Joback Method
dvisc	0.0000950	Pa×s	660.50	Joback Method
dvisc	0.0001611	Pa×s	594.31	Joback Method
dvisc	0.0003119	Pa×s	528.13	Joback Method
dvisc	0.0007296	Pa×s	461.94	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=U356062&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

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