

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:	ONRCGOHVXOTDPZ-AATRIKPKSA-N
Formula:	C22H40O4
SMILES:	CCC=CCCOC(=O)CCCCCCCC(=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
rinpola	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000617	Paxs	726.69	Joback Method
dvisc	0.0000950	Paxs	660.50	Joback Method
dvisc	0.0001611	Paxs	594.31	Joback Method
dvisc	0.0003119	Paxs	528.13	Joback Method
dvisc	0.0007296	Paxs	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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