

Sebacic acid, isoheptyl 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)CCCCCCCC(=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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000436	Paxs	759.41	Joback Method
dvisc	0.0000695	Paxs	686.93	Joback Method
dvisc	0.0001238	Paxs	614.45	Joback Method
dvisc	0.0002572	Paxs	541.96	Joback Method
dvisc	0.0006695	Paxs	469.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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