

Sebacic acid, nonyl pent-4-en-2-yl ester

Inchi:	InChI=1S/C24H44O4/c1-4-6-7-8-11-14-17-21-27-23(25)19-15-12-9-10-13-16-20-24(26)2
InchiKey:	PWKPWUQOAOTEGA-UHFFFAOYSA-N
Formula:	C24H44O4
SMILES:	C=CCC(C)OC(=O)CCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	396.60

Physical Properties

Property code	Value	Unit	Source
gf	-231.24	kJ/mol	Joback Method
hf	-908.14	kJ/mol	Joback Method
hfus	58.69	kJ/mol	Joback Method
hvap	86.27	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.909		Crippen Method
mvol	359.600	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	2680.00		NIST Webbook
tb	897.34	K	Joback Method
tc	1098.99	K	Joback Method
tf	487.80	K	Joback Method
vc	1.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.12	J/molxK	897.34	Joback Method
cpg	1273.70	J/molxK	1065.38	Joback Method
cpg	1259.31	J/molxK	1031.78	Joback Method
cpg	1243.69	J/molxK	998.17	Joback Method
cpg	1226.81	J/molxK	964.56	Joback Method
cpg	1208.64	J/molxK	930.95	Joback Method
cpg	1286.91	J/molxK	1098.99	Joback Method
dvisc	0.0000289	Paxs	897.34	Joback Method
dvisc	0.0000391	Paxs	829.08	Joback Method

dvisc	0.0000557	Paxs	760.83	Joback Method
dvisc	0.0000852	Paxs	692.57	Joback Method
dvisc	0.0001429	Paxs	624.31	Joback Method
dvisc	0.0002724	Paxs	556.06	Joback Method
dvisc	0.0006217	Paxs	487.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355956&Units=SI

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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