

Carbonic acid, nonyl prop-1-en-2-yl ester

Inchi:	InChI=1S/C13H24O3/c1-4-5-6-7-8-9-10-11-15-13(14)16-12(2)3/h2,4-11H2,1,3H3
InchiKey:	JELOZNAWSKWMGG-UHFFFAOYSA-N
Formula:	C13H24O3
SMILES:	<chem>C=C(C)OC(=O)OCCCCCCCCC</chem>
Mol. weight [g/mol]:	228.33

Physical Properties

Property code	Value	Unit	Source
gf	-201.05	kJ/mol	Joback Method
hf	-573.03	kJ/mol	Joback Method
hfus	30.81	kJ/mol	Joback Method
hvap	55.51	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.424		Crippen Method
mvol	203.040	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
tb	592.11	K	Joback Method
tc	765.66	K	Joback Method
tf	314.94	K	Joback Method
vc	0.787	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.06	J/mol×K	592.11	Joback Method
cpg	537.83	J/mol×K	621.03	Joback Method
cpg	552.96	J/mol×K	649.96	Joback Method
cpg	567.45	J/mol×K	678.88	Joback Method
cpg	581.31	J/mol×K	707.81	Joback Method
cpg	594.54	J/mol×K	736.73	Joback Method
cpg	607.15	J/mol×K	765.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382539&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/90-857-1/Carbonic-acid-nonyl-prop-1-en-2-yl-ester.pdf>

Generated by Cheméo on 2024-04-18 02:49:32.00248211 +0000 UTC m=+15697820.923059433.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.