

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H30O3/c1-4-5-6-7-8-9-10-11-12-13-14-18-16(17)19-15(2)3/h2,4-14H2,1,3H

YNTFFRYKXYSRHC-UHFFFAOYSA-N

C16H30O3

C=C(C)OC(=O)OCCCCCCCCCCCCC

270.41

Physical Properties

Property code	Value	Unit	Source
gf	-175.79	kJ/mol	Joback Method
hf	-634.95	kJ/mol	Joback Method
hfus	38.58	kJ/mol	Joback Method
hvap	62.19	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.594		Crippen Method
mcvol	245.310	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
tb	660.75	K	Joback Method
tc	832.43	K	Joback Method
tf	348.75	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.07	J/mol×K	660.75	Joback Method
cpg	700.42	J/mol×K	689.36	Joback Method
cpg	717.01	J/mol×K	717.98	Joback Method
cpg	732.84	J/mol×K	746.59	Joback Method
cpg	747.94	J/mol×K	775.20	Joback Method
cpg	762.30	J/mol×K	803.81	Joback Method
cpg	775.94	J/mol×K	832.43	Joback Method

Sources

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=U382907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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