

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C17H32O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-17(18)20-16(2)3/h2,4-15H2,1

FIEQVBIWRHOKBE-UHFFFAOYSA-N

C17H32O3

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

284.43

Physical Properties

Property code	Value	Unit	Source
gf	-167.37	kJ/mol	Joback Method
hf	-655.59	kJ/mol	Joback Method
hfus	41.17	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.984		Crippen Method
mcvol	259.400	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	1892.00		NIST Webbook
rinpol	1892.00		NIST Webbook
tb	683.63	K	Joback Method
tc	855.45	K	Joback Method
tf	360.02	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.42	J/mol×K	683.63	Joback Method
cpg	757.22	J/mol×K	712.27	Joback Method
cpg	774.21	J/mol×K	740.90	Joback Method
cpg	790.41	J/mol×K	769.54	Joback Method
cpg	805.84	J/mol×K	798.18	Joback Method
cpg	820.50	J/mol×K	826.82	Joback Method
cpg	834.41	J/mol×K	855.45	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=U382908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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