2,2-Dimethylpropanoic acid, undec-2-enyl ester

Inchi: InChI=1S/C16H30O2/c1-5-6-7-8-9-10-11-12-13-14-18-15(17)16(2,3)4/h12-13H,5-11,14H

InchiKey: CUCZIHQHCUDPKZ-OUKQBFOZSA-N

Formula: C16H30O2

SMILES: CCCCCCCCC=CCOC(=O)C(C)(C)C

Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
gf	-67.02	kJ/mol	Joback Method
hf	-509.90	kJ/mol	Joback Method
hfus	32.77	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.883		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tb	642.70	K	Joback Method
tc	822.27	K	Joback Method
tf	339.58	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.63	J/mol×K	642.70	Joback Method
cpg	675.70	J/mol×K	672.63	Joback Method
cpg	692.88	J/mol×K	702.56	Joback Method
cpg	709.20	J/mol×K	732.49	Joback Method
cpg	724.71	J/mol×K	762.42	Joback Method
cpg	739.43	J/mol×K	792.35	Joback Method
cpg	753.41	J/mol×K	822.27	Joback Method
dvisc	0.0025532	Pa×s	339.58	Joback Method

dvisc	0.0010215	Pa×s	390.10	Joback Method
dvisc	0.0005042	Pa×s	440.62	Joback Method
dvisc	0.0002878	Pa×s	491.14	Joback Method
dvisc	0.0001824	Pa×s	541.66	Joback Method
dvisc	0.0001249	Pa×s	592.18	Joback Method
dvisc	0.0000908	Pa×s	642.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U299337&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