11-(2-Cyclopentenyl)undecanoic acid, ethyl ester

Other names: Ethyl hydnocarpate
Hydnocarpic acid, ethyl ester
ethyl 11-cyclopent-2-enylundecanoate

Inchi: InChI=1S/C18H32O2/c1-2-20-18(19)16-10-8-6-4-3-5-7-9-13-17-14-11-12-15-17/h11,14,1

InchiKey: IXHZJQBOONNARJ-UHFFFAOYSA-N

Formula: C18H32O2

SMILES: CCOC(=O)CCCCCCCCCCC1C=CCC1

Mol. weight [g/mol]: 280.45

CAS: 3552-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-66.73	kJ/mol	Joback Method
hf	-541.39	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.417		Crippen Method
mcvol	256.760	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
rinpol	2051.40		NIST Webbook
rinpol	2051.40		NIST Webbook
tb	701.97	K	Joback Method
tc	886.18	K	Joback Method
tf	376.44	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.72	J/mol×K	701.97	Joback Method
cpg	778.11	J/mol×K	732.67	Joback Method
cpg	796.48	J/mol×K	763.37	Joback Method
cpg	813.87	J/mol×K	794.08	Joback Method

cpg	830.31	J/mol×K	824.78	Joback Method
cpg	845.83	J/mol×K	855.48	Joback Method
cpg	860.46	J/mol×K	886.18	Joback Method
dvisc	0.0021457	Pa×s	376.44	Joback Method
dvisc	0.0010315	Pa×s	430.69	Joback Method
dvisc	0.0005842	Pa×s	484.95	Joback Method
dvisc	0.0003710	Pa×s	539.20	Joback Method
dvisc	0.0002560	Pa×s	593.46	Joback Method
dvisc	0.0001879	Pa×s	647.71	Joback Method
dvisc	0.0001447	Pa×s	701.97	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=C3552123&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

Latest version available from: