11-(2-Cyclopenten-1-yl)undecanoic acid, (+)-

Other names: Hydnocarpic acid
2-Cyclopentene-1-undecanoic acid
Isolated from chaulmoogra oil
Inchi: InChI=1S/C16H28O2/c17-16(18)14-8-6-4-2-1-3-5-7-11-15-12-9-10-13-15/h9,12,15H,1-8,
InchiKey: SRELFLQJDOTNLJ-UHFFFAOYSA-N
Formula: C16H28O2
SMILES: O=C(O)CCCCCCCCCCC1C=CCC1
Mol. weight [g/mol]: 252.39
CAS: 459-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-115.39	kJ/mol	Joback Method
hf	-520.12	kJ/mol	Joback Method
hfus	38.04	kJ/mol	Joback Method
hvap	75.18	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.938		Crippen Method
mcvol	228.580	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2025.70		NIST Webbook
rinpol	2025.70		NIST Webbook
tb	725.97	K	Joback Method
tc	908.40	K	Joback Method
tf	392.49	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.62	J/mol×K	725.97	Joback Method
cpg	702.79	J/mol×K	756.38	Joback Method
cpg	718.10	J/mol×K	786.78	Joback Method
cpg	732.59	J/mol×K	817.19	Joback Method

cpg	746.29	J/mol×K	847.59	Joback Method
cpg	759.24	J/mol×K	878.00	Joback Method
cpg	771.49	J/mol×K	908.40	Joback Method
dvisc	0.0035172	Pa×s	392.49	Joback Method
dvisc	0.0011282	Pa×s	448.07	Joback Method
dvisc	0.0004651	Pa×s	503.65	Joback Method
dvisc	0.0002287	Pa×s	559.23	Joback Method
dvisc	0.0001278	Pa×s	614.81	Joback Method
dvisc	0.0000787	Pa×s	670.39	Joback Method
dvisc	0.0000522	Pa×s	725.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C459676&Units=SI
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

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

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