

12-hexadecenol, E

Other names:	(E)12-Hexadecen-1-ol
Inchi:	InChI=1S/C16H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h4-5,17H,2-3,6-16H2,1
InchiKey:	QTZQYQLPKOVNSX-SNAWJCMRSA-N
Formula:	C16H32O
SMILES:	CCCC=CCCCCCCCCCCCCO
Mol. weight [g/mol]:	240.42

Physical Properties

Property code	Value	Unit	Source
gf	27.24	kJ/mol	Joback Method
hf	-408.58	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	67.85	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.236		Crippen Method
mcvol	237.870	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	1877.00		NIST Webbook
ripol	2422.00		NIST Webbook
tb	661.82	K	Joback Method
tc	825.49	K	Joback Method
tf	325.82	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.38	J/mol×K	661.82	Joback Method
cpg	687.84	J/mol×K	689.10	Joback Method
cpg	703.60	J/mol×K	716.38	Joback Method
cpg	718.68	J/mol×K	743.66	Joback Method
cpg	733.13	J/mol×K	770.94	Joback Method
cpg	746.95	J/mol×K	798.21	Joback Method
cpg	760.19	J/mol×K	825.49	Joback Method

dvisc	0.0083536	Pa×s	325.82	Joback Method
dvisc	0.0017184	Pa×s	381.82	Joback Method
dvisc	0.0005297	Pa×s	437.82	Joback Method
dvisc	0.0002133	Pa×s	493.82	Joback Method
dvisc	0.0001033	Pa×s	549.82	Joback Method
dvisc	0.0000572	Pa×s	605.82	Joback Method
dvisc	0.0000351	Pa×s	661.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R77749&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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