

E-2-HEXADECACEN-1-OL

Other names:	2-hexadecen-1-ol
Inchi:	InChI=1S/C16H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h14-15,17H,2-13,16H2
InchiKey:	MIDSQDHRRBSMIZ-CCEZHUSRSA-N
Formula:	C16H32O
SMILES:	CCCCCCCCCCCCC/C=C/CO
Mol. weight [g/mol]:	240.43
CAS:	---

Physical Properties

Property code	Value	Unit	Source
af	0.9031		Cheméo Relay (1.0)
gf	27.24	kJ/mol	Joback Method
hf	-438.12	kJ/mol	Cheméo Relay (1.0)
hfus	41.49	kJ/mol	Joback Method
hvap	108.94	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-6.26		Cheméo Relay (1.0)
logp	5.236		Crippen Method
mcvol	237.870	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
ripol	2574.00		NIST Webbook
ripol	2574.00		NIST Webbook
tb	585.56	K	Cheméo Relay (1.0)
tc	769.32	K	Cheméo Relay (1.0)
tf	319.13	K	Cheméo Relay (1.0)
vc	0.896	m3/kmol	Cheméo Relay (1.0)

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42406e+01
Coeff. B	-4.94719e+03
Coeff. C	-1.07158e+02
Temperature range (K), min.	461.72
Temperature range (K), max.	661.21

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U131101&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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