

(10E,12Z)-hexadecandien-1-ol

Inchi:	InChI=1S/C16H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h4-7,17H,2-3,8-16H2,1
InchiKey:	CIVIWCVVOFNUST-SCFJQAPRSA-N
Formula:	C16H30O
SMILES:	CCCC=CC=CCCCCCCCCO
Mol. weight [g/mol]:	238.41
CAS:	1002-94-4

Physical Properties

Property code	Value	Unit	Source
gf	107.46	kJ/mol	Joback Method
hf	-291.36	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	67.81	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.012		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	1919.00		NIST Webbook
tb	665.98	K	Joback Method
tc	833.90	K	Joback Method
tf	320.74	K	Joback Method
vc	0.910	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.91	J/molxK	665.98	Joback Method
cpg	665.88	J/molxK	693.97	Joback Method
cpg	681.15	J/molxK	721.95	Joback Method
cpg	695.75	J/molxK	749.94	Joback Method
cpg	709.70	J/molxK	777.93	Joback Method
cpg	723.06	J/molxK	805.91	Joback Method
cpg	735.86	J/molxK	833.90	Joback Method
dvisc	0.0083725	Paxs	320.74	Joback Method

dvisc	0.0016004	Paxs	378.28	Joback Method
dvisc	0.0004736	Paxs	435.82	Joback Method
dvisc	0.0001862	Paxs	493.36	Joback Method
dvisc	0.0000889	Paxs	550.90	Joback Method
dvisc	0.0000489	Paxs	608.44	Joback Method
dvisc	0.0000298	Paxs	665.98	Joback Method

Sources

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=C1002944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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