1,5-HEXADIEN-3-OL

Other names:	1,5-Hexadiene-3-ol
	hexa-1,5-dien-3-ol
Inchi:	InChI=1S/C6H10O/c1-3-5-6(7)4-2/h3-4,6-7H,1-2,5H2
InchiKey:	SZYLTIUVWARXOO-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C=CCC(O)C=C
Mol. weight [g/mol]:	98.14
CAS:	924-41-4

Physical Properties

Property code	Value	Unit	Source
af	0.4920		Cheméo Relay (1.0)
hf	-145.70	kJ/mol	Cheméo Relay (1.0)
hfus	9.30	kJ/mol	Joback Method
hvap	52.79	kJ/mol	Cheméo Relay (1.0)
ie	9.66	eV	Cheméo Relay (1.0)
log10ws	-0.26		Cheméo Relay (1.0)
logp	1.109		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	406.70	K	NIST Webbook
tc	576.97	K	Cheméo Relay (1.0)
tf	199.74	K	Cheméo Relay (1.0)
vc	0.329	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.91	J/mol×K	421.78	Joback Method
cpg	185.46	J/mol×K	450.30	Joback Method
cpg	193.63	J/mol×K	478.82	Joback Method
cpg	201.42	J/mol×K	507.34	Joback Method
cpg	208.84	J/mol×K	535.86	Joback Method
cpg	215.92	J/mol×K	564.39	Joback Method

cpg	222.66	J/mol×K	592.91	Joback Method
dvisc	0.1801344	Pa×s	199.68	Joback Method
dvisc	0.0253750	Pa×s	236.70	Joback Method
dvisc	0.0060735	Pa×s	273.71	Joback Method
dvisc	0.0020437	Pa×s	310.73	Joback Method
dvisc	0.0008672	Pa×s	347.75	Joback Method
dvisc	0.0004339	Pa×s	384.76	Joback Method
dvisc	0.0002452	Pa×s	421.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	315.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59642e+01
Coeff. B	-3.99944e+03
Coeff. C	-5.41990e+01
Temperature range (K), min.	309.32
Temperature range (K), max.	429.64

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C924414&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/ci990307l

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

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume