1,6-Heptadien-4-ol

Other names: hepta-1,6-dien-4-ol
Inchi: InChI=1S/C7H12O/c1-3-5-7(8)6-4-2/h3-4,7-8H,1-2,5-6H2
InchiKey: UTGFOWQYZKTZTN-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C=CCC(O)CC=C
Mol. weight [g/mol]: 112.17
CAS: 2883-45-6

Physical Properties

Property code	Value	Unit	Source
gf	44.48	kJ/mol	Joback Method
hf	-94.46	kJ/mol	Joback Method
hfus	11.89	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.499		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	876.00		NIST Webbook
ripol	1330.00		NIST Webbook
tb	424.20	K	NIST Webbook
tc	614.77	K	Joback Method
tf	210.95	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.43	J/mol×K	444.66	Joback Method
cpg	225.11	J/mol×K	473.01	Joback Method
cpg	234.36	J/mol×K	501.36	Joback Method
cpg	243.19	J/mol×K	529.72	Joback Method
cpg	251.62	J/mol×K	558.07	Joback Method
cpg	259.65	J/mol×K	586.42	Joback Method

cpg	267.31	J/mol×K	614.77	Joback Method
dvisc	0.1349769	Pa×s	210.95	Joback Method
dvisc	0.0198157	Pa×s	249.90	Joback Method
dvisc	0.0048808	Pa×s	288.85	Joback Method
dvisc	0.0016772	Pa×s	327.81	Joback Method
dvisc	0.0007231	Pa×s	366.76	Joback Method
dvisc	0.0003664	Pa×s	405.71	Joback Method
dvisc	0.0002092	Pa×s	444.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59627e+01
Coeff. B	-4.14225e+03
Coeff. C	-5.90640e+01
Temperature range (K), min.	323.32
Temperature range (K), max.	447.96

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=C2883456&Units=SI

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor 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