3,5-Hexadien-2-ol

Inchi: InChI=1S/C6H10O/c1-3-4-5-6(2)7/h3-7H,1H2,2H3/b5-4+
InchiKey: VAOJQRMYAXTUQI-SNAWJCMRSA-N
Formula: C6H10O
SMILES: C=CC=CC(C)O
Mol. weight [g/mol]: 98.14
CAS: 3280-51-1

Physical Properties

Property code	Value	Unit	Source
gf	28.44	kJ/mol	Joback Method
hf	-82.03	kJ/mol	Joback Method
hfus	10.78	kJ/mol	Joback Method
hvap	44.53	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.109		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
rinpol	775.00		NIST Webbook
rinpol	786.00		NIST Webbook
tb	429.26	K	Joback Method
tc	605.20	K	Joback Method
tf	196.36	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.33	J/mol×K	429.26	Joback Method
cpg	185.12	J/mol×K	458.58	Joback Method
cpg	193.47	J/mol×K	487.91	Joback Method
cpg	201.40	J/mol×K	517.23	Joback Method
cpg	208.92	J/mol×K	546.55	Joback Method
cpg	216.06	J/mol×K	575.88	Joback Method
cpg	222.84	J/mol×K	605.20	Joback Method

dvisc	0.2199580	Pa×s	196.36	Joback Method
dvisc	0.0259231	Pa×s	235.18	Joback Method
dvisc	0.0055996	Pa×s	273.99	Joback Method
dvisc	0.0017693	Pa×s	312.81	Joback Method
dvisc	0.0007210	Pa×s	351.63	Joback Method
dvisc	0.0003512	Pa×s	390.44	Joback Method
dvisc	0.0001948	Pa×s	429.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56104e+01
Coeff. B	-3.88524e+03
Coeff. C	-5.33670e+01
Temperature range (K), min.	306.93
Temperature range (K), max.	430.62

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3280511&Units=SI

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

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