1,5-octadien-3-ol

Other names: octa-1,5-dien-3-ol
Inchi: InChI=1S/C8H14O/c1-3-5-6-7-8(9)4-2/h4-6,8-9H,2-3,7H2,1H3/b6-5+
InchiKey: APFBWMGEGSELQP-AATRIKPKSA-N
Formula: C8H14O
SMILES: C=CC(O)CC=CCC
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
gf	45.28	kJ/mol	Joback Method
hf	-123.31	kJ/mol	Joback Method
hfus	15.96	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.890		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	965.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	977.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1357.00		NIST Webbook
tb	475.02	K	Joback Method
tc	648.36	K	Joback Method
tf	218.90	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	256.29	J/mol×K	475.02	Joback Method
cpg	267.19	J/mol×K	503.91	Joback Method
cpg	277.57	J/mol×K	532.80	Joback Method
cpg	287.45	J/mol×K	561.69	Joback Method
cpg	296.85	J/mol×K	590.58	Joback Method
cpg	305.80	J/mol×K	619.47	Joback Method
cpg	314.32	J/mol×K	648.36	Joback Method
dvisc	0.1182924	Pa×s	218.90	Joback Method
dvisc	0.0154310	Pa×s	261.59	Joback Method
dvisc	0.0035647	Pa×s	304.27	Joback Method
dvisc	0.0011810	Pa×s	346.96	Joback Method
dvisc	0.0004984	Pa×s	389.65	Joback Method
dvisc	0.0002494	Pa×s	432.33	Joback Method
dvisc	0.0001413	Pa×s	475.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R211508&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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

Latest version available from:

https://www.chemeo.com/cid/40-476-9/1-5-octadien-3-ol.pdf

Generated by Cheméo on 2024-04-27 16:58:22.34153069 +0000 UTC m=+16526351.262108054.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.