4-Methyl-1,6-heptadien-4-ol

Other names:	1,6-Heptadien-4-ol, 4-methyl-
	4-Methyl-1,6-heptadiene-4-ol
	4-methylhepta-1,6-dien-4-ol
	Diallyl methyl carbinol
Inchi:	InChI=1S/C8H14O/c1-4-6-8(3,9)7-5-2/h4-5,9H,1-2,6-7H2,3H3
InchiKey:	WAXJJHZQRWWQIR-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	C=CCC(C)(O)CC=C
Mol. weight [g/mol]:	126.20
CAS:	25201-40-5

Physical Properties

Property code	Value	Unit	Source
gf	58.18	kJ/mol	Joback Method
hf	-118.57	kJ/mol	Joback Method
hfus	10.59	kJ/mol	Joback Method
hvap	47.45	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.890		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	464.75	K	Joback Method
tc	640.18	K	Joback Method
tf	239.64	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.82	J/mol×K	464.75	Joback Method
cpg	309.89	J/mol×K	610.94	Joback Method
cpg	300.80	J/mol×K	581.71	Joback Method
cpg	291.17	J/mol×K	552.47	Joback Method
cpg	280.98	J/mol×K	523.23	Joback Method

cpg	270.21	J/mol×K	493.99	Joback Method
cpg	318.49	J/mol×K	640.18	Joback Method
dvisc	0.0001903	Pa×s	464.75	Joback Method
dvisc	0.0003287	Pa×s	427.23	Joback Method
dvisc	0.0006309	Pa×s	389.71	Joback Method
dvisc	0.0013914	Pa×s	352.19	Joback Method
dvisc	0.0037057	Pa×s	314.68	Joback Method
dvisc	0.0128662	Pa×s	277.16	Joback Method
dvisc	0.0659635	Pa×s	239.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36714e+01
Coeff. B	-3.58846e+03
Coeff. C	-6.11210e+01
Temperature range (K), min.	329.24
Temperature range (K), max.	490.37

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=C25201405&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
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/11-150-2/4-Methyl-1-6-heptadien-4-ol.pdf

Generated by Cheméo on 2024-10-12 03:41:34.073915904 +0000 UTC m=+3285356.710885152.

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