

4-Allyl-1,6-heptadiene-4-ol

Other names:	4-Allyl-1,6-heptadien-4-ol Triallylcarbinol
Inchi:	InChI=1S/C10H16O/c1-4-7-10(11,8-5-2)9-6-3/h4-6,11H,1-3,7-9H2
InchiKey:	SUXQWOWVXDXQSE-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C=CCC(O)(CC=C)CC=C
Mol. weight [g/mol]:	152.23
CAS:	10202-75-2

Physical Properties

Property code	Value	Unit	Source
gf	162.86	kJ/mol	Joback Method
hf	-34.42	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	51.23	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.446		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1069.00		NIST Webbook
tb	507.19	K	Joback Method
tc	682.99	K	Joback Method
tf	260.42	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.05	J/mol×K	507.19	Joback Method
cpg	340.51	J/mol×K	536.49	Joback Method
cpg	352.29	J/mol×K	565.79	Joback Method
cpg	363.41	J/mol×K	595.09	Joback Method
cpg	373.92	J/mol×K	624.39	Joback Method
cpg	383.84	J/mol×K	653.69	Joback Method

cpg	393.22	J/mol×K	682.99	Joback Method
dvisc	0.0375298	Pa×s	260.42	Joback Method
dvisc	0.0077307	Pa×s	301.55	Joback Method
dvisc	0.0023268	Pa×s	342.68	Joback Method
dvisc	0.0009059	Pa×s	383.81	Joback Method
dvisc	0.0004233	Pa×s	424.93	Joback Method
dvisc	0.0002263	Pa×s	466.06	Joback Method
dvisc	0.0001339	Pa×s	507.19	Joback Method

Sources

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=C10202752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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