

1,6-Heptadien-4-ol, 4-propyl-

Other names:	4-Propyl-1,6-heptadien-4-ol
Inchi:	InChI=1S/C10H18O/c1-4-7-10(11,8-5-2)9-6-3/h4-5,11H,1-2,6-9H2,3H3
InchiKey:	UPDFVVLBKBYBOG-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=CCC(O)(CC=C)CCC
Mol. weight [g/mol]:	154.25
CAS:	52939-61-4

Physical Properties

Property code	Value	Unit	Source
gf	75.02	kJ/mol	Joback Method
hf	-159.85	kJ/mol	Joback Method
hfus	15.77	kJ/mol	Joback Method
hvap	51.90	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.670		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
tb	510.51	K	Joback Method
tc	683.12	K	Joback Method
tf	262.18	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.36	J/mol×K	510.51	Joback Method
cpg	405.08	J/mol×K	654.35	Joback Method
cpg	394.55	J/mol×K	625.58	Joback Method
cpg	383.44	J/mol×K	596.81	Joback Method
cpg	371.73	J/mol×K	568.05	Joback Method
cpg	359.38	J/mol×K	539.28	Joback Method
cpg	415.06	J/mol×K	683.12	Joback Method
dvisc	0.0001293	Pa×s	510.51	Joback Method

dvisc	0.0002202	Pa×s	469.12	Joback Method
dvisc	0.0004158	Pa×s	427.73	Joback Method
dvisc	0.0008997	Pa×s	386.35	Joback Method
dvisc	0.0023429	Pa×s	344.96	Joback Method
dvisc	0.0079203	Pa×s	303.57	Joback Method
dvisc	0.0393328	Pa×s	262.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52939614&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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