3,4-Hexadien-2-ol, 3-isopropenyl-2,5-dimethyl-

Other names: 3-Isopropenyl-2,5-dimethyl-3,4-hexadien-2-ol
3,4-Hexadien-2-ol, 2,5-dimethyl-3-(1-methylethenyl)
Inchi: InChI=1S/C11H18O/c1-8(2)7-10(9(3)4)11(5,6)12/h12H,3H2,1-2,4-6H3
InchiKey: OOYJYXZAXCOHEW-UHFFFAOYSA-N
Formula: C11H18O
SMILES: C=C(C)C(=C=C(C)C)C(C)(C)O
Mol. weight [g/mol]: 166.26
CAS: 15448-75-6

Physical Properties

Property code	Value	Unit	Source
gf	178.45	kJ/mol	Joback Method
hf	-55.29	kJ/mol	Joback Method
hfus	18.04	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.825		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	543.78	K	Joback Method
tc	737.66	K	Joback Method
tf	234.76	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.28	J/mol×K	543.78	Joback Method
cpg	391.23	J/mol×K	576.09	Joback Method
cpg	404.40	J/mol×K	608.41	Joback Method
cpg	416.83	J/mol×K	640.72	Joback Method
cpg	428.57	J/mol×K	673.03	Joback Method

cpg	439.66	J/mol×K	705.35	Joback Method
cpg	450.14	J/mol×K	737.66	Joback Method

Sources

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=C15448756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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