(2E,4E)-2,4-Dimethyl-2,4-hexadien-1-ol

Inchi: InChI=1S/C8H14O/c1-4-7(2)5-8(3)6-9/h4-5,9H,6H2,1-3H3/b7-4+,8-5+
InchiKey: YZDKYYZSTTWZDN-NSLJXJERSA-N
Formula: C8H14O
SMILES: CC=C(C)C=C(C)CO
Mol. weight [g/mol]: 126.20

Physical Properties

Property code	Value	Unit	Source
gf	23.00	kJ/mol	Joback Method
hf	-145.82	kJ/mol	Joback Method
hfus	18.35	kJ/mol	Joback Method
hvap	50.16	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.891		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1058.00		NIST Webbook
rinpol	1058.00		NIST Webbook
tb	482.70	K	Joback Method
tc	663.05	K	Joback Method
tf	202.66	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.05	J/mol×K	482.70	Joback Method
cpg	267.16	J/mol×K	512.76	Joback Method
cpg	277.68	J/mol×K	542.82	Joback Method
cpg	287.66	J/mol×K	572.87	Joback Method
cpg	297.13	J/mol×K	602.93	Joback Method
cpg	306.12	J/mol×K	632.99	Joback Method
cpg	314.66	J/mol×K	663.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R597634&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
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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