1,7-Nonadien-4-ol, 4,8-dimethyl-

Other names: 4,8-Dimethyl-1,7-nonadien-4-ol
Inchi: InChI=1S/C11H20O/c1-5-8-11(4,12)9-6-7-10(2)3/h5,7,12H,1,6,8-9H2,2-4H3
InchiKey: PWEXDCWJSFTGOP-UHFFFAOYSA-N
Formula: C11H20O
SMILES: C=CCC(C)(O)CCC=C(C)C
Mol. weight [g/mol]: 168.28
CAS: 17920-92-2

Physical Properties

Property code	Value	Unit	Source
gf	67.27	kJ/mol	Joback Method
hf	-198.49	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.060		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1191.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
tb	540.75	K	Joback Method
tc	718.76	K	Joback Method
tf	256.17	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.73	J/mol×K	540.75	Joback Method
cpg	407.75	J/mol×K	570.42	Joback Method
cpg	421.02	J/mol×K	600.09	Joback Method
cpg	433.57	J/mol×K	629.75	Joback Method
cpg	445.46	J/mol×K	659.42	Joback Method

cpg	456.72	J/mol×K	689.09	Joback Method
cpg	467.40	J/mol×K	718.76	Joback Method

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=C17920922&Units=SI

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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