

3,7-Nonadien-2-ol, 4,8-dimethyl-

Other names:	4,8-Dimethyl-3,7-nonadien-2-ol 4,8-Dimethylnona-3,7-dien-2-ol
Inchi:	InChI=1S/C11H20O/c1-9(2)6-5-7-10(3)8-11(4)12/h6,8,11-12H,5,7H2,1-4H3/b10-8+
InchiKey:	NYPOJSCNHYZRG-CSKARUKUSA-N
Formula:	C11H20O
SMILES:	CC(C)=CCCC(C)=CC(C)O
Mol. weight [g/mol]:	168.28
CAS:	67845-50-5

Physical Properties

Property code	Value	Unit	Source
gf	45.82	kJ/mol	Joback Method
hf	-213.02	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	56.45	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.060		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1329.00		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1311.00		NIST Webbook
tb	550.90	K	Joback Method
tc	729.66	K	Joback Method
tf	221.47	K	Joback Method
vc	0.626	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.66	J/molxK	550.90	Joback Method
cpg	405.48	J/molxK	580.69	Joback Method
cpg	418.62	J/molxK	610.49	Joback Method
cpg	431.12	J/molxK	640.28	Joback Method

cpg	443.00	J/mol×K	670.08	Joback Method
cpg	454.31	J/mol×K	699.87	Joback Method
cpg	465.08	J/mol×K	729.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67845505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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