(E)-2,6-Dimethylnona-6,8-dien-4-ol

Inchi: InChI=1S/C11H20O/c1-5-6-10(4)8-11(12)7-9(2)3/h5-6,9,11-12H,1,7-8H2,2-4H3/b10-6+
InchiKey: NTRAMYHXCXBYEN-UXBLZVDNSA-N
Formula: C11H20O
SMILES: C=CC=C(C)CC(O)CC(C)C
Mol. weight [g/mol]: 168.28

Physical Properties

Property code	Value	Unit	Source
gf	59.55	kJ/mol	Joback Method
hf	-200.30	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	55.35	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.916		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1222.00		NIST Webbook
rinpol	1222.00		NIST Webbook
tb	543.10	K	Joback Method
tc	718.44	K	Joback Method
tf	223.75	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.17	J/mol×K	543.10	Joback Method
cpg	405.00	J/mol×K	572.32	Joback Method
cpg	418.17	J/mol×K	601.55	Joback Method
cpg	430.70	J/mol×K	630.77	Joback Method
cpg	442.64	J/mol×K	659.99	Joback Method
cpg	454.01	J/mol×K	689.22	Joback Method
cpg	464.84	J/mol×K	718.44	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=R232070&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