

1,8-NONADIENE, 2-METHYL-5,7-DIMETHYLENE-

Other names:	2-Methyl-5,7-dimethylene-1,8-nonadiene
Inchi:	InChI=1S/C12H18/c1-6-11(4)9-12(5)8-7-10(2)3/h6H,1-2,4-5,7-9H2,3H3
InchiKey:	RCZAYHKXHPHPX-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	C=CC(=C)CC(=C)CCC(=C)C
Mol. weight [g/mol]:	162.28

Physical Properties

Property code	Value	Unit	Source
hf	123.93	kJ/mol	Cheméo Relay (1.0)
hfus	17.79	kJ/mol	Joback Method
hvap	54.11	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
logp	4.031		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
tb	459.30	K	Cheméo Relay (1.0)
tf	213.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.50	J/mol×K	460.32	Joback Method
cpg	352.12	J/mol×K	490.85	Joback Method
cpg	366.96	J/mol×K	521.37	Joback Method
cpg	381.04	J/mol×K	551.90	Joback Method
cpg	394.40	J/mol×K	582.42	Joback Method
cpg	407.08	J/mol×K	612.95	Joback Method
cpg	419.11	J/mol×K	643.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U152688&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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