

dimethyl-2,9 decadiene-1,9

Inchi:

lnchl=1S/C12H22/c1-11(2)9-7-5-6-8-10-12(3)4/h1,3,5-10H2,2,4H3

InchiKey:

BEJQIHUHGNTYQT-UHFFFAOYSA-N

Formula:

C12H22

SMILES:

C=C(C)CCCCCCC(=C)C

Mol. weight [g/mol]:

166.30

Physical Properties

Property code	Value	Unit	Source
gf	208.74	kJ/mol	Joback Method
hf	-59.73	kJ/mol	Joback Method
hfus	21.66	kJ/mol	Joback Method
hvap	41.13	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.479		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
ripol	1346.00		NIST Webbook
ripol	1346.00		NIST Webbook
tb	467.08	K	Joback Method
tc	639.98	K	Joback Method
tf	193.56	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.21	J/mol×K	467.08	Joback Method
cpg	387.56	J/mol×K	495.90	Joback Method
cpg	403.21	J/mol×K	524.71	Joback Method
cpg	418.18	J/mol×K	553.53	Joback Method
cpg	432.49	J/mol×K	582.34	Joback Method
cpg	446.16	J/mol×K	611.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=R242527&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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