

# 3,4-dimethyl-6-ethyl-octane, a

Inchi:	InChI=1S/C12H26/c1-6-10(4)11(5)9-12(7-2)8-3/h10-12H,6-9H2,1-5H3
InchiKey:	DPDGQUZDZYGOBAM-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCC(CC)CC(C)C(C)CC
Mol. weight [g/mol]:	170.33

## Physical Properties

Property code	Value	Unit	Source
gf	42.84	kJ/mol	Joback Method
hf	-306.85	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	41.14	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.495		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinsol	1101.00		NIST Webbook
tb	472.64	K	Joback Method
tc	643.64	K	Joback Method
tf	180.00	K	Joback Method
vc	0.690	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.03	J/molxK	472.64	Joback Method
cpg	490.12	J/molxK	615.14	Joback Method
cpg	474.87	J/molxK	586.64	Joback Method
cpg	458.95	J/molxK	558.14	Joback Method
cpg	442.35	J/molxK	529.64	Joback Method
cpg	425.05	J/molxK	501.14	Joback Method
cpg	504.72	J/molxK	643.64	Joback Method
dvisc	0.0001829	Paxs	472.64	Joback Method
dvisc	0.0002670	Paxs	423.87	Joback Method

dvisc	0.0004300	Paxs	375.09	Joback Method
dvisc	0.0007987	Paxs	326.32	Joback Method
dvisc	0.0018440	Paxs	277.55	Joback Method
dvisc	0.0060831	Paxs	228.77	Joback Method
dvisc	0.0383167	Paxs	180.00	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R173367&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R173367&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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