

1,7-Octadiene, 2,4-dimethyl-3-chloro-

Inchi:	InChI=1S/C10H17Cl/c1-5-6-7-9(4)10(11)8(2)3/h5,9-10H,1-2,6-7H2,3-4H3
InchiKey:	AXODEFMWRIJEFZ-UHFFFAOYSA-N
Formula:	C10H17Cl
SMILES:	C=CCCC(C)C(Cl)C(=C)C
Mol. weight [g/mol]:	172.69

Physical Properties

Property code	Value	Unit	Source
gf	183.64	kJ/mol	Joback Method
hf	-34.96	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	40.20	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.772		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
tb	457.99	K	Joback Method
tc	644.57	K	Joback Method
tf	184.90	K	Joback Method
vc	0.596	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.47	J/mol×K	457.99	Joback Method
cpg	329.13	J/mol×K	489.09	Joback Method
cpg	343.06	J/mol×K	520.18	Joback Method
cpg	356.31	J/mol×K	551.28	Joback Method
cpg	368.89	J/mol×K	582.38	Joback Method
cpg	380.84	J/mol×K	613.48	Joback Method
cpg	392.18	J/mol×K	644.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=B6010335&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/63-833-7/1-7-Octadiene-2-4-dimethyl-3-chloro.pdf>

Generated by Cheméo on 2024-05-01 00:38:24.453198001 +0000 UTC m=+16813153.373775322.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.