

2,3-Dimethyl-2-octene

Other names:	n-C ₅ H ₁₁ C(CH ₃)=C(CH ₃) ₂ 2-Octene, 2,3-dimethyl
Inchi:	InChI=1S/C10H20/c1-5-6-7-8-10(4)9(2)3/h5-8H2,1-4H3
InchiKey:	ZFMOZNIUEPVNVCV-UHFFFAOYSA-N
Formula:	C ₁₀ H ₂₀
SMILES:	CCCCC(C)=C(C)C
Mol. weight [g/mol]:	140.27
CAS:	19781-18-1

Physical Properties

Property code	Value	Unit	Source
gf	96.44	kJ/mol	Joback Method
hf	-152.09	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	37.97	kJ/mol	Joback Method
ie	8.13 ± 0.01	eV	NIST Webbook
log10ws	-3.86		Crippen Method
logp	3.923		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	961.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	959.00		NIST Webbook
tb	441.90 ± 1.50	K	NIST Webbook
tb	442.30 ± 1.50	K	NIST Webbook
tb	441.90 ± 2.00	K	NIST Webbook
tc	608.78	K	Joback Method
tf	187.00 ± 2.00	K	NIST Webbook
tf	187.20 ± 2.00	K	NIST Webbook
vc	0.578	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.15	J/mol×K	432.12	Joback Method
cpg	315.61	J/mol×K	461.56	Joback Method
cpg	330.39	J/mol×K	491.01	Joback Method
cpg	344.52	J/mol×K	520.45	Joback Method
cpg	358.03	J/mol×K	549.89	Joback Method
cpg	370.94	J/mol×K	579.34	Joback Method
cpg	383.26	J/mol×K	608.78	Joback Method

Sources

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=C19781181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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

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