

3-OCTENE, 2,2-DIMETHYL-

Other names:	2,2-dimethyl-3-octene
Inchi:	InChI=1S/C10H20/c1-5-6-7-8-9-10(2,3)4/h8-9H,5-7H2,1-4H3/b9-8+
InchiKey:	PWMYBNEYORINWQV-CMDGGOBGSA-N
Formula:	C10H20
SMILES:	CCCC/C=C/C(C)(C)C
Mol. weight [g/mol]:	140.27
CAS:	19482-57-6

Physical Properties

Property code	Value	Unit	Source
af	0.3290		Cheméo Relay (1.0)
gf	116.38	kJ/mol	Joback Method
hf	-133.29	kJ/mol	Cheméo Relay (1.0)
hfus	14.44	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-5.18		Cheméo Relay (1.0)
logp	3.779		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
tb	411.21	K	Cheméo Relay (1.0)
tc	581.12	K	Cheméo Relay (1.0)
tf	165.53	K	Cheméo Relay (1.0)
vc	0.549	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.13	J/mol×K	429.13	Joback Method
cpg	318.57	J/mol×K	459.30	Joback Method
cpg	334.17	J/mol×K	489.47	Joback Method
cpg	348.96	J/mol×K	519.65	Joback Method
cpg	362.99	J/mol×K	549.82	Joback Method
cpg	376.28	J/mol×K	579.99	Joback Method

cpg	388.89	J/mol×K	610.16	Joback Method
dvisc	0.0104937	Pa×s	199.80	Joback Method
dvisc	0.0032229	Pa×s	238.02	Joback Method
dvisc	0.0013722	Pa×s	276.24	Joback Method
dvisc	0.0007191	Pa×s	314.47	Joback Method
dvisc	0.0004334	Pa×s	352.69	Joback Method
dvisc	0.0002885	Pa×s	390.91	Joback Method
dvisc	0.0002064	Pa×s	429.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50118e+01
Coeff. B	-3.92429e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	328.92
Temperature range (K), max.	466.95

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C86869763&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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