

2-Octene, 2,6-dimethyl-

Other names:	2,6-Dimethyl-2-octene 2,6-Dimethyl-oct-2-ene
Inchi:	InChI=1S/C10H20/c1-5-10(4)8-6-7-9(2)3/h7,10H,5-6,8H2,1-4H3
InchiKey:	WQNLWKDARWVSKE-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CCC(C)CCC=C(C)C
Mol. weight [g/mol]:	140.27
CAS:	4057-42-5

Physical Properties

Property code	Value	Unit	Source
gf	102.55	kJ/mol	Joback Method
hf	-147.58	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	37.50	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.779		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	967.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	967.00		NIST Webbook
tb	431.80	K	Joback Method
tc	609.06	K	Joback Method
tf	168.42	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.23	J/mol×K	431.80	Joback Method
cpg	315.85	J/mol×K	461.34	Joback Method
cpg	330.80	J/mol×K	490.89	Joback Method
cpg	345.08	J/mol×K	520.43	Joback Method

cpg	358.72	J/mol×K	549.97	Joback Method
cpg	371.75	J/mol×K	579.52	Joback Method
cpg	384.19	J/mol×K	609.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46876e+01
Coeff. B	-3.80190e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	326.42
Temperature range (K), max.	467.89

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4057425&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

pvap:	Vapor 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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