2,2-Dimethyloctane

Other names: Octane, 2,2-dimethyl-
Inchi: InChI=1S/C10H22/c1-5-6-7-8-9-10(2,3)4/h5-9H2,1-4H3
InchiKey: GPBUTTSWJNPYJL-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCCCCCC(C)(C)C
Mol. weight [g/mol]: 142.29
CAS: 15869-87-1

Physical Properties

Property code	Value	Unit	Source
af	0.4125		Cheméo Relay (1.0)
gf	36.16	kJ/mol	Joback Method
hf	-266.11	kJ/mol	Cheméo Relay (1.0)
hfus	14.24	kJ/mol	Joback Method
hvap	49.00	kJ/mol	NIST Webbook
ie	9.48	eV	Cheméo Relay (1.0)
log10ws	-5.79		Cheméo Relay (1.0)
logp	4.003		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	917.60		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	918.70		NIST Webbook
rinpol	918.70		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	918.10		NIST Webbook
rinpol	914.90		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	922.80		NIST Webbook

rinpol	919.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	920.30		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	922.80		NIST Webbook
tb	427.83	K	Cheméo Relay (1.0)
tc	588.69	K	Cheméo Relay (1.0)
tf	196.14	K	Cheméo Relay (1.0)
vc	0.571	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.97	J/mol×K	424.97	Joback Method
cpg	333.53	J/mol×K	453.73	Joback Method
cpg	349.34	J/mol×K	482.48	Joback Method
cpg	364.44	J/mol×K	511.24	Joback Method
cpg	378.86	J/mol×K	539.99	Joback Method
cpg	392.61	J/mol×K	568.75	Joback Method
cpg	405.72	J/mol×K	597.50	Joback Method
dvisc	0.0108562	Pa×s	204.88	Joback Method
dvisc	0.0035911	Pa×s	241.56	Joback Method
dvisc	0.0015903	Pa×s	278.24	Joback Method
dvisc	0.0008514	Pa×s	314.92	Joback Method
dvisc	0.0005192	Pa×s	351.61	Joback Method
dvisc	0.0003477	Pa×s	388.29	Joback Method
dvisc	0.0002495	Pa×s	424.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43929e+01
Coeff. B	-3.68888e+03
Coeff. C	-5.26550e+01
Temperature range (K), min.	314.18
Temperature range (K), max.	458.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.24663e+01
Coeff. B	-7.79653e+03
Coeff. C	-8.31381e+00
Coeff. D	3.74626e-06
Temperature range (K), min.	225.00
Temperature range (K), max.	602.00

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0, beta):

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=104

KDB: https://www.cheric.org/files/research/kdb/mol/mol104.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869871&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume