

Decane, 2,2-dimethyl-

Other names:	2,2-Dimethyldecane
Inchi:	InChI=1S/C12H26/c1-5-6-7-8-9-10-11-12(2,3)4/h5-11H2,1-4H3
InchiKey:	WBWYXWILSHQILH-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCCCCCCC(C)(C)C
Mol. weight [g/mol]:	170.33
CAS:	17302-37-3

Physical Properties

Property code	Value	Unit	Source
gf	53.00	kJ/mol	Joback Method
hf	-299.76	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	41.01	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.783		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1114.00		NIST Webbook
tb	470.73	K	Joback Method
tc	640.99	K	Joback Method
tf	227.42	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.96	J/molxK	470.73	Joback Method
cpg	427.03	J/molxK	499.11	Joback Method
cpg	444.30	J/molxK	527.48	Joback Method

cpg	460.79	J/mol×K	555.86	Joback Method
cpg	476.54	J/mol×K	584.24	Joback Method
cpg	491.58	J/mol×K	612.61	Joback Method
cpg	505.93	J/mol×K	640.99	Joback Method
dvisc	0.0097058	Paxs	227.42	Joback Method
dvisc	0.0031716	Paxs	267.97	Joback Method
dvisc	0.0013906	Paxs	308.52	Joback Method
dvisc	0.0007385	Paxs	349.07	Joback Method
dvisc	0.0004474	Paxs	389.63	Joback Method
dvisc	0.0002979	Paxs	430.18	Joback Method
dvisc	0.0002128	Paxs	470.73	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39349e+01
Coeff. B	-3.56672e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	352.66
Temperature range (K), max.	504.92

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C17302373&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/75-364-5/Decane-2-2-dimethyl.pdf>

Generated by Cheméo on 2024-04-26 09:48:53.626412417 +0000 UTC m=+16414182.546989733.

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