

Decane, 2,9-dimethyl-

Other names:	2,9-Dimethyldecane
Inchi:	InChI=1S/C12H26/c1-11(2)9-7-5-6-8-10-12(3)4/h11-12H,5-10H2,1-4H3
InchiKey:	HWISDPDDDUZJAW-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CC(C)CCCCCCC(C)C
Mol. weight [g/mol]:	170.33
CAS:	1002-17-1

Physical Properties

Property code	Value	Unit	Source
gf	45.28	kJ/mol	Joback Method
hf	-301.57	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	41.53	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
tb	473.08	K	Joback Method
tc	640.63	K	Joback Method
tf	195.00	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.97	J/molxK	473.08	Joback Method
cpg	424.55	J/molxK	501.00	Joback Method
cpg	441.45	J/molxK	528.93	Joback Method
cpg	457.68	J/molxK	556.85	Joback Method

cpg	473.26	J/mol×K	584.78	Joback Method
cpg	488.21	J/mol×K	612.70	Joback Method
cpg	502.54	J/mol×K	640.63	Joback Method
dvisc	0.0185767	Paxs	195.00	Joback Method
dvisc	0.0041744	Paxs	241.35	Joback Method
dvisc	0.0015175	Paxs	287.69	Joback Method
dvisc	0.0007305	Paxs	334.04	Joback Method
dvisc	0.0004202	Paxs	380.39	Joback Method
dvisc	0.0002726	Paxs	426.73	Joback Method
dvisc	0.0001925	Paxs	473.08	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40732e+01
Coeff. B	-3.64801e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	355.94
Temperature range (K), max.	507.67

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1002171&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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