

Nonane, 4,5-dimethyl-

Other names:	4,5-Dimethylnonane 5,6-Dimethyl-nonane
Inchi:	InChI=1S/C11H24/c1-5-7-9-11(4)10(3)8-6-2/h10-11H,5-9H2,1-4H3
InchiKey:	JDNGDDOTBYZAGS-UHFFFAOYSA-N
Formula:	C11H24
SMILES:	CCCCC(C)C(C)CCC
Mol. weight [g/mol]:	156.31
CAS:	17302-23-7

Physical Properties

Property code	Value	Unit	Source
gf	36.86	kJ/mol	Joback Method
hf	-280.93	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	39.30	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.249		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1035.00		NIST Webbook
tb	450.20	K	Joback Method
tc	618.81	K	Joback Method
tf	183.73	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.12	J/molxK	450.20	Joback Method
cpg	376.92	J/molxK	478.30	Joback Method
cpg	393.08	J/molxK	506.40	Joback Method
cpg	408.60	J/molxK	534.51	Joback Method
cpg	423.51	J/molxK	562.61	Joback Method
cpg	437.81	J/molxK	590.71	Joback Method

cpg	451.53	J/molxK	618.81	Joback Method
dvisc	0.0200727	Paxs	183.73	Joback Method
dvisc	0.0044499	Paxs	228.14	Joback Method
dvisc	0.0016118	Paxs	272.55	Joback Method
dvisc	0.0007760	Paxs	316.96	Joback Method
dvisc	0.0004471	Paxs	361.38	Joback Method
dvisc	0.0002907	Paxs	405.79	Joback Method
dvisc	0.0002057	Paxs	450.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40076e+01
Coeff. B	-3.47121e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	338.45
Temperature range (K), max.	484.62

Sources

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=C17302237&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

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
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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