2,4-Dimethylnonane

Other names: Nonane, 2,4-dimethyl
Inchi: InChI=1S/C11H24/c1-5-6-7-8-11(4)9-10(2)3/h10-11H,5-9H2,1-4H3
InchiKey: JZUUOAUSQCXSTN-UHFFFAOYSA-N
Formula: C11H24
SMILES: CCCCCC(C)CC(C)C
Mol. weight [g/mol]: 156.31
CAS: 17302-24-8

Physical Properties

Property code	Value	Unit	Source
af	0.4607		Cheméo Relay (1.0)
gf	36.86	kJ/mol	Joback Method
hf	-287.19	kJ/mol	Cheméo Relay (1.0)
hfus	17.20	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-6.04		Cheméo Relay (1.0)
logp	4.249		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
tb	445.25	K	Cheméo Relay (1.0)
tc	610.54	K	Cheméo Relay (1.0)
tf	190.39	K	Cheméo Relay (1.0)
vc	0.619	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.81	J/mol×K	590.71	Joback Method
cpg	451.53	J/mol×K	618.81	Joback Method
cpg	376.92	J/mol×K	478.30	Joback Method
cpg	393.08	J/mol×K	506.40	Joback Method
cpg	408.60	J/mol×K	534.51	Joback Method
cpg	423.51	J/mol×K	562.61	Joback Method

cpg	360.12	J/mol×K	450.20	Joback Method
dvisc	0.0016118	Pa×s	272.55	Joback Method
dvisc	0.0044499	Pa×s	228.14	Joback Method
dvisc	0.0200727	Pa×s	183.73	Joback Method
dvisc	0.0007760	Pa×s	316.96	Joback Method
dvisc	0.0004471	Pa×s	361.38	Joback Method
dvisc	0.0002907	Pa×s	405.79	Joback Method
dvisc	0.0002057	Pa×s	450.20	Joback Method
hvapt	46.80	kJ/mol	393.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39944e+01
Coeff. B	-3.42884e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	335.61
Temperature range (K), max.	480.34

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17302248&Units=SI

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

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

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume