2,2-dimethylnonane

Inchi: InChI=1S/C11H24/c1-5-6-7-8-9-10-11(2,3)4/h5-10H2,1-4H3
InchiKey: WDSBVMLUILIJOW-UHFFFAOYSA-N
Formula: C11H24
SMILES: CCCCCCCC(C)(C)C
Mol. weight [g/mol]: 156.31
CAS: 17302-14-6

Physical Properties

Property code	Value	Unit	Source
af	0.4572		Cheméo Relay (1.0)
gf	44.58	kJ/mol	Joback Method
hf	-287.84	kJ/mol	Cheméo Relay (1.0)
hfus	16.83	kJ/mol	Joback Method
hvap	49.40	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
log10ws	-6.19		Cheméo Relay (1.0)
logp	4.393		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
tb	450.06	K	Cheméo Relay (1.0)
tc	610.72	K	Cheméo Relay (1.0)
tf	209.21	K	Cheméo Relay (1.0)
vc	0.631	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.00	J/mol×K	447.85	Joback Method
cpg	379.36	J/mol×K	476.42	Joback Method
cpg	395.95	J/mol×K	505.00	Joback Method
cpg	411.80	J/mol×K	533.57	Joback Method
cpg	426.92	J/mol×K	562.14	Joback Method
cpg	441.36	J/mol×K	590.71	Joback Method
cpg	455.13	J/mol×K	619.29	Joback Method

dvisc	0.0103350	Pa×s	216.15	Joback Method
dvisc	0.0033968	Pa×s	254.77	Joback Method
dvisc	0.0014964	Pa×s	293.38	Joback Method
dvisc	0.0007977	Pa×s	332.00	Joback Method
dvisc	0.0004848	Pa×s	370.62	Joback Method
dvisc	0.0003237	Pa×s	409.23	Joback Method
dvisc	0.0002317	Pa×s	447.85	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38705e+01
Coeff. B	-3.40203e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	335.91
Temperature range (K), max.	482.93

Sources

Cheméo Relay (1.0, beta):

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=C17302146&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):

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume