Nonane, 2,2,3-trimethyl-

Other names: 2,2,3-Trimethylnonane
Inchi: InChI=1S/C12H26/c1-6-7-8-9-10-11(2)12(3,4)5/h11H,6-10H2,1-5H3
InchiKey: XXNUJUNKYOZLAJ-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCCCCC(C)C(C)(C)C
Mol. weight [g/mol]: 170.33
CAS: 55499-04-2

Physical Properties

Property code	Value	Unit	Source
gf	50.56	kJ/mol	Joback Method
hf	-305.04	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	40.62	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1114.00		NIST Webbook
tb	470.29	K	Joback Method
tc	644.11	K	Joback Method
tf	212.42	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.02	J/mol×K	470.29	Joback Method
cpg	427.54	J/mol×K	499.26	Joback Method
cpg	445.22	J/mol×K	528.23	Joback Method
cpg	462.09	J/mol×K	557.20	Joback Method
cpg	478.18	J/mol×K	586.17	Joback Method
cpg	493.52	J/mol×K	615.14	Joback Method
cpg	508.14	J/mol×K	644.11	Joback Method

dvisc	0.0170934	Pa×s	212.42	Joback Method
dvisc	0.0043803	Pa×s	255.40	Joback Method
dvisc	0.0016616	Pa×s	298.38	Joback Method
dvisc	0.0008046	Pa×s	341.36	Joback Method
dvisc	0.0004582	Pa×s	384.33	Joback Method
dvisc	0.0002922	Pa×s	427.31	Joback Method
dvisc	0.0002023	Pa×s	470.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38156e+01
Coeff. B	-3.51185e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	350.91
Temperature range (K), max.	504.27

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55499042&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/ci990307l

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

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