Nonane, 3,3-dimethyl

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

Physical Properties

Property code	Value	Unit	Source
gf	44.58	kJ/mol	Joback Method
hf	-279.12	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.393		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1030.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	1030.00		NIST Webbook
tb	447.85	K	Joback Method
tc	619.29	K	Joback Method
tf	216.15	K	Joback Method
vc	0.640	m3/kmol	Joback Method

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

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R71274&Units=SI

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
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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