2,4,6-Trimethyl-1-nonene, # 1

Other names: 1-Nonene, 2,4,6-trimethyl, # 1
Inchi: InChI=1S/C12H24/c1-6-7-11(4)9-12(5)8-10(2)3/h11-12H,2,6-9H2,1,3-5H3
InchiKey: QFMQAIUZMMQKTB-UHFFFAOYSA-N
Formula: C12H24
SMILES: C=C(C)CC(C)CC(C)CCC
Mol. weight [g/mol]: 168.32

Physical Properties

Property code	Value	Unit	Source
gf	124.57	kJ/mol	Joback Method
hf	-185.93	kJ/mol	Joback Method
hfus	17.20	kJ/mol	Joback Method
hvap	40.94	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.415		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1070.00		NIST Webbook
rinpol	1082.00		NIST Webbook
tb	469.64	K	Joback Method
tc	643.38	K	Joback Method
tf	179.28	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.06	J/mol×K	469.64	Joback Method
cpg	406.47	J/mol×K	498.60	Joback Method
cpg	423.15	J/mol×K	527.55	Joback Method
cpg	439.12	J/mol×K	556.51	Joback Method
cpg	454.41	J/mol×K	585.47	Joback Method
cpg	469.02	J/mol×K	614.42	Joback Method
cpg	482.99	J/mol×K	643.38	Joback Method

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=R529641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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