

2,5,8-Trimethyl-1-nonene

Inchi:	InChI=1S/C12H24/c1-10(2)6-8-12(5)9-7-11(3)4/h11-12H,1,6-9H2,2-5H3
InchiKey:	QACSSVAYGPHMJG-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	C=C(C)CCC(C)CCC(C)C
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
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/molxK	469.64	Joback Method
cpg	406.47	J/molxK	498.60	Joback Method
cpg	423.15	J/molxK	527.55	Joback Method
cpg	439.12	J/molxK	556.51	Joback Method
cpg	454.41	J/molxK	585.47	Joback Method
cpg	469.02	J/molxK	614.42	Joback Method
cpg	482.99	J/molxK	643.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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