

Octane, 2,6,6-trimethyl-

Inchi:	InChI=1S/C11H24/c1-6-11(4,5)9-7-8-10(2)3/h10H,6-9H2,1-5H3
InchiKey:	RUPXAIGHLDMSOL-UHFFFAOYSA-N
Formula:	C11H24
SMILES:	CCC(C)(C)CCCC(C)C
Mol. weight [g/mol]:	156.31
CAS:	54166-32-4

Physical Properties

Property code	Value	Unit	Source
gf	42.14	kJ/mol	Joback Method
hf	-284.40	kJ/mol	Joback Method
hfus	13.31	kJ/mol	Joback Method
hvap	38.40	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.249		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
tb	447.41	K	Joback Method
tc	622.57	K	Joback Method
tf	201.15	K	Joback Method
vc	0.634	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.01	J/molxK	447.41	Joback Method
cpg	379.83	J/molxK	476.60	Joback Method
cpg	396.84	J/molxK	505.80	Joback Method
cpg	413.06	J/molxK	534.99	Joback Method
cpg	428.53	J/molxK	564.18	Joback Method
cpg	443.27	J/molxK	593.38	Joback Method
cpg	457.31	J/molxK	622.57	Joback Method
dvisc	0.0188587	Paxs	201.15	Joback Method
dvisc	0.0047986	Paxs	242.19	Joback Method

dvisc	0.0018154	Paxs	283.24	Joback Method
dvisc	0.0008784	Paxs	324.28	Joback Method
dvisc	0.0005003	Paxs	365.32	Joback Method
dvisc	0.0003193	Paxs	406.37	Joback Method
dvisc	0.0002213	Paxs	447.41	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=C54166324&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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