

Octane, 2,3,6-trimethyl-

Other names:	2,3,6-Trimethyl-octane
Inchi:	InChI=1S/C11H24/c1-6-10(4)7-8-11(5)9(2)3/h9-11H,6-8H2,1-5H3
InchiKey:	MNFBUNLEXRMWOY-UHFFFAOYSA-N
Formula:	C11H24
SMILES:	CCC(C)CCC(C)C(C)C
Mol. weight [g/mol]:	156.31
CAS:	62016-33-5

Physical Properties

Property code	Value	Unit	Source
gf	34.42	kJ/mol	Joback Method
hf	-286.21	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	38.92	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	4.105		Crippen Method
mcvol	165.850	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
tb	449.76	K	Joback Method
tc	621.98	K	Joback Method
tf	168.73	K	Joback Method
vc	0.633	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.14	J/mol×K	449.76	Joback Method
cpg	377.38	J/mol×K	478.46	Joback Method
cpg	393.94	J/mol×K	507.17	Joback Method
cpg	409.83	J/mol×K	535.87	Joback Method
cpg	425.08	J/mol×K	564.57	Joback Method
cpg	439.69	J/mol×K	593.28	Joback Method
cpg	453.69	J/mol×K	621.98	Joback Method
dvisc	0.0437057	Paxs	168.73	Joback Method

dvisc	0.0066714	Paxs	215.57	Joback Method
dvisc	0.0019921	Paxs	262.41	Joback Method
dvisc	0.0008579	Paxs	309.25	Joback Method
dvisc	0.0004611	Paxs	356.08	Joback Method
dvisc	0.0002863	Paxs	402.92	Joback Method
dvisc	0.0001963	Paxs	449.76	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=C62016335&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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