

Octane, 2,3,6,7-tetramethyl-

Inchi:	InChI=1S/C12H26/c1-9(2)11(5)7-8-12(6)10(3)4/h9-12H,7-8H2,1-6H3
InchiKey:	FZCGYGZYRXL DY-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CC(C)C(C)CCC(C)C(C)C
Mol. weight [g/mol]:	170.33
CAS:	52670-34-5

Physical Properties

Property code	Value	Unit	Source
gf	40.40	kJ/mol	Joback Method
hf	-312.13	kJ/mol	Joback Method
hfus	12.74	kJ/mol	Joback Method
hvap	40.75	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	4.351		Crippen Method
mvol	179.940	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
tb	472.20	K	Joback Method
tc	646.78	K	Joback Method
tf	165.00	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.10	J/molxK	472.20	Joback Method
cpg	492.09	J/molxK	617.68	Joback Method
cpg	476.52	J/molxK	588.59	Joback Method
cpg	460.26	J/molxK	559.49	Joback Method
cpg	443.29	J/molxK	530.39	Joback Method
cpg	425.57	J/molxK	501.30	Joback Method
cpg	506.97	J/molxK	646.78	Joback Method
dvisc	0.0001738	Paxs	472.20	Joback Method
dvisc	0.0002619	Paxs	421.00	Joback Method

dvisc	0.0004420	Paxs	369.80	Joback Method
dvisc	0.0008827	Paxs	318.60	Joback Method
dvisc	0.0022975	Paxs	267.40	Joback Method
dvisc	0.0094069	Paxs	216.20	Joback Method
dvisc	0.0923748	Paxs	165.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52670345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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