Octane, 2,3,7-trimethyl-

Inchi: InChI=1S/C11H24/c1-9(2)7-6-8-11(5)10(3)4/h9-11H,6-8H2,1-5H3
InchiKey: XJKKSYAVEVAGFX-UHFFFAOYSA-N
Formula: C11H24
SMILES: CC(C)CCCC(C)C(C)C
Mol. weight [g/mol]: 156.31
CAS: 62016-34-6

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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.14	J/mol×K	449.76	Joback Method
cpg	439.69	J/mol×K	593.28	Joback Method
cpg	425.08	J/mol×K	564.57	Joback Method
cpg	409.83	J/mol×K	535.87	Joback Method
cpg	393.94	J/mol×K	507.17	Joback Method
cpg	377.38	J/mol×K	478.46	Joback Method
cpg	453.69	J/mol×K	621.98	Joback Method
dvisc	0.0001963	Pa×s	449.76	Joback Method
dvisc	0.0002863	Pa×s	402.92	Joback Method

dvisc	0.0004611	Pa×s	356.08	Joback Method
dvisc	0.0008579	Pa×s	309.25	Joback Method
dvisc	0.0019921	Pa×s	262.41	Joback Method
dvisc	0.0066714	Pa×s	215.57	Joback Method
dvisc	0.0437057	Pa×s	168.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62016346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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