Octane, 2,4,6-trimethyl-

Other names: 2,4,6-Trimethyl-octane
Inchi: InChI=1S/C11H24/c1-6-10(4)8-11(5)7-9(2)3/h9-11H,6-8H2,1-5H3
InchiKey: XHNIFDXYGLPJLP-UHFFFAOYSA-N
Formula: C11H24
SMILES: CCC(C)CC(C)CC(C)C
Mol. weight [g/mol]: 156.31
CAS: 62016-37-9

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
rinpol	955.00		NIST Webbook
rinpol	955.00		NIST Webbook
ripol	1058.00		NIST Webbook
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	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	Pa×s	168.73	Joback Method
dvisc	0.0066714	Pa×s	215.57	Joback Method
dvisc	0.0019921	Pa×s	262.41	Joback Method
dvisc	0.0008579	Pa×s	309.25	Joback Method
dvisc	0.0004611	Pa×s	356.08	Joback Method
dvisc	0.0002863	Pa×s	402.92	Joback Method
dvisc	0.0001963	Pa×s	449.76	Joback Method
hvapt	44.90	kJ/mol	383.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62016379&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

hvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

rinpol: Non-polar retention indices

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume