Octane, 2,3,3-trimethyl-

Inchi: InChI=1S/C11H24/c1-6-7-8-9-11(4,5)10(2)3/h10H,6-9H2,1-5H3
InchiKey: KFYWDCDWVPXXCA-UHFFFAOYSA-N
Formula: C11H24
SMILES: CCCCCC(C)(C)C(C)C
Mol. weight [g/mol]: 156.31
CAS: 62016-30-2

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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0018154	Pa×s	283.24	Joback Method
dvisc	0.0008784	Pa×s	324.28	Joback Method
dvisc	0.0005003	Pa×s	365.32	Joback Method
dvisc	0.0003193	Pa×s	406.37	Joback Method
dvisc	0.0002213	Pa×s	447.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62016302&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

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