Octane, 2,2,6-trimethyl-

Other names: 2,2,6-Trimethyloctane
Inchi: InChI=1S/C11H24/c1-6-10(2)8-7-9-11(3,4)5/h10H,6-9H2,1-5H3
InchiKey: NBIHFQKVSFKHGH-UHFFFAOYSA-N
Formula: C11H24
SMILES: CCC(C)CCCC(C)(C)C
Mol. weight [g/mol]: 156.31
CAS: 62016-28-8

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37335e+01
Coeff. B	-3.29695e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	330.65
Temperature range (K), max.	476.92

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62016288&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume