4,4-Dimethyl octane

Other names:	4,4-DIMETHYLOCTANE
	Octane, 4,4-dimethyl-
Inchi:	InChI=1S/C10H22/c1-5-7-9-10(3,4)8-6-2/h5-9H2,1-4H3
InchiKey:	ZMEDGZAGMLTROM-UHFFFAOYSA-N
Formula:	C10H22
SMILES:	CCCCC(C)(C)CCC
Mol. weight [g/mol]:	142.28
CAS:	15869-95-1

Physical Properties

Property code	Value	Unit	Source
gf	36.16	kJ/mol	Joback Method
hf	-258.48	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	48.10	kJ/mol	NIST Webbook
log10ws	-3.77		Crippen Method
logp	4.003		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	920.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	918.00		NIST Webbook

rinpol	918.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	920.00		NIST Webbook
tb	430.65 ± 0.50	K	NIST Webbook
tb	426.15 ± 3.00	K	NIST Webbook
tb	428.00 ± 2.00	K	NIST Webbook
tb	430.70	K	NIST Webbook
tc	597.50	K	Joback Method
tf	204.88	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.97	J/mol×K	424.97	Joback Method
cpg	333.53	J/mol×K	453.73	Joback Method
cpg	349.34	J/mol×K	482.48	Joback Method
cpg	364.44	J/mol×K	511.24	Joback Method
cpg	378.86	J/mol×K	539.99	Joback Method
cpg	392.61	J/mol×K	568.75	Joback Method
cpg	405.72	J/mol×K	597.50	Joback Method
dvisc	0.0108562	Pa×s	204.88	Joback Method
dvisc	0.0035911	Pa×s	241.56	Joback Method
dvisc	0.0015903	Pa×s	278.24	Joback Method
dvisc	0.0008514	Pa×s	314.92	Joback Method
dvisc	0.0005192	Pa×s	351.61	Joback Method
dvisc	0.0003477	Pa×s	388.29	Joback Method
dvisc	0.0002495	Pa×s	424.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.00564e+02
Coeff. B	-8.97438e+03
Coeff. C	-1.26107e+01
Coeff. D	7.43125e-06

Temperature range (K), min.	315.15
Temperature range (K), max.	606.90

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15869951&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=114
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol114.mol

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume