3,4,5,6-Tetramethyloctane, a

Inchi: InChI=1S/C12H26/c1-7-9(3)11(5)12(6)10(4)8-2/h9-12H,7-8H2,1-6H3
InchiKey: NADJQGPTQSFIHB-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCC(C)C(C)C(C)C(C)CC
Mol. weight [g/mol]: 170.33

Physical Properties

Property code	Value	Unit	Source
gf	40.40	kJ/mol	Joback Method
hf	-312.13	kJ/mol	Joback Method
hfus	12.74	kJ/mol	Joback Method
hvap	40.75	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	4.351		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	1100.60		NIST Webbook
rinpol	1100.60		NIST Webbook
tb	472.20	K	Joback Method
tc	646.78	K	Joback Method
tf	165.00	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.10	J/mol×K	472.20	Joback Method
cpg	425.57	J/mol×K	501.30	Joback Method
cpg	443.29	J/mol×K	530.39	Joback Method
cpg	460.26	J/mol×K	559.49	Joback Method
cpg	476.52	J/mol×K	588.59	Joback Method
cpg	492.09	J/mol×K	617.68	Joback Method
cpg	506.97	J/mol×K	646.78	Joback Method
dvisc	0.0923748	Pa×s	165.00	Joback Method

dvisc	0.0094069	Pa×s	216.20	Joback Method
dvisc	0.0022975	Pa×s	267.40	Joback Method
dvisc	0.0008827	Pa×s	318.60	Joback Method
dvisc	0.0004420	Pa×s	369.80	Joback Method
dvisc	0.0002619	Pa×s	421.00	Joback Method
dvisc	0.0001738	Pa×s	472.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R173238&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume