2,2,4,4-Tetramethyloctane

Inchi: InChI=1S/C12H26/c1-7-8-9-12(5,6)10-11(2,3)4/h7-10H2,1-6H3
InchiKey: TYUFTNSABIBNRY-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCCC(C)(C)CC(C)(C)C
Mol. weight [g/mol]: 170.33
CAS: 62183-79-3

Physical Properties

Property code	Value	Unit	Source
gf	55.84	kJ/mol	Joback Method
hf	-308.51	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	39.71	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
tb	467.50	K	Joback Method
tc	648.06	K	Joback Method
tf	229.84	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.01	J/mol×K	467.50	Joback Method
cpg	430.55	J/mol×K	497.59	Joback Method
cpg	449.07	J/mol×K	527.69	Joback Method
cpg	466.62	J/mol×K	557.78	Joback Method
cpg	483.25	J/mol×K	587.87	Joback Method
cpg	498.99	J/mol×K	617.96	Joback Method
cpg	513.90	J/mol×K	648.06	Joback Method
dvisc	0.0149911	Pa×s	229.84	Joback Method
dvisc	0.0043865	Pa×s	269.45	Joback Method

dvisc	0.0017587	Pa×s	309.06	Joback Method
dvisc	0.0008679	Pa×s	348.67	Joback Method
dvisc	0.0004947	Pa×s	388.28	Joback Method
dvisc	0.0003129	Pa×s	427.89	Joback Method
dvisc	0.0002139	Pa×s	467.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35485e+01
Coeff. B	-3.33842e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	343.06
Temperature range (K), max.	496.61

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62183793&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

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