2,2,3,3-Tetramethyloctane

Inchi: InChI=1S/C12H26/c1-7-8-9-10-12(5,6)11(2,3)4/h7-10H2,1-6H3
InchiKey: UXQAEOWCSOPBLF-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCCCC(C)(C)C(C)(C)C
Mol. weight [g/mol]: 170.33
CAS: 62183-74-8

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
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
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	1.35734e+01
Coeff. B	-3.41938e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	348.68
Temperature range (K), max.	505.18

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=R505249&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume