3,3,6,6-Tetramethyloctane

Inchi: InChI=1S/C12H26/c1-7-11(3,4)9-10-12(5,6)8-2/h7-10H2,1-6H3
InchiKey: PAEUGKMMSQUAGH-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCC(C)(C)CCC(C)(C)CC
Mol. weight [g/mol]: 170.33
CAS: 62199-46-6

Physical Properties

Property code	Value	Unit	Source
chl	-8065.10	kJ/mol	NIST Webbook
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	462.90 ± 0.60	K	NIST Webbook
tc	648.06	K	Joback Method
tf	199.56 ± 0.20	K	NIST Webbook
tf	199.87 ± 0.10	K	NIST Webbook
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.90	J/mol×K	648.06	Joback Method
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

dvisc	0.0002139	Pa×s	467.50	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
hvapt	52.90	kJ/mol	405.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62199466&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume