Hexane, 3,4-bis(1,1-dimethylethyl)-2,2,5,5-tetramethyl-

Other names: 1,1,2,2-Tetra-t-butylethane
Inchi: InChI=1S/C18H38/c1-15(2,3)13(16(4,5)6)14(17(7,8)9)18(10,11)12/h13-14H,1-12H3
InchiKey: RMASWOHNLWIUPT-UHFFFAOYSA-N
Formula: C18H38
SMILES: CC(C)(C)C(C(C(C)(C)C)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 254.49
CAS: 62850-21-9

Physical Properties

Property code	Value	Unit	Source
chs	-12189.00 ± 4.00	kJ/mol	NIST Webbook
gf	107.16	kJ/mol	Joback Method
hf	-251.00 ± 4.00	kJ/mol	NIST Webbook
hfs	-325.00 ± 4.00	kJ/mol	NIST Webbook
hfus	5.67	kJ/mol	Joback Method
hsub	74.00	kJ/mol	NIST Webbook
hsub	74.30	kJ/mol	NIST Webbook
hvap	49.70	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	6.403		Crippen Method
mcvol	264.480	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
tb	597.44	K	Joback Method
tc	794.00	K	Joback Method
tf	272.30	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.51	J/mol×K	761.24	Joback Method
cpg	823.26	J/mol×K	728.48	Joback Method
cpg	802.77	J/mol×K	695.72	Joback Method
cpg	780.93	J/mol×K	662.96	Joback Method

cpg	757.65	J/mol×K	630.20	Joback Method
cpg	732.81	J/mol×K	597.44	Joback Method
cpg	860.62	J/mol×K	794.00	Joback Method
dvisc	0.0298051	Pa×s	272.30	Joback Method
dvisc	0.0000681	Pa×s	597.44	Joback Method
dvisc	0.0001131	Pa×s	543.25	Joback Method
dvisc	0.0002104	Pa×s	489.06	Joback Method
dvisc	0.0004570	Pa×s	434.87	Joback Method
dvisc	0.0012373	Pa×s	380.68	Joback Method
dvisc	0.0046636	Pa×s	326.49	Joback Method
hsubt	74.27 ± 0.54	kJ/mol	303.00	NIST Webbook
hsubt	71.90	kJ/mol	334.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62850219&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

chs: Standard solid 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
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume