3-Hexene, 2,5-dimethyl-3,4-bis(1-methylethyl)-

Inchi: InChI=1S/C14H28/c1-9(2)13(10(3)4)14(11(5)6)12(7)8/h9-12H,1-8H3
InchiKey: CHUZFFSJMAKRES-UHFFFAOYSA-N
Formula: C14H28
SMILES: CC(C)C(=C(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 196.37
CAS: 7090-88-2

Physical Properties

Property code	Value	Unit	Source
gf	120.36	kJ/mol	Joback Method
hf	-255.77	kJ/mol	Joback Method
hfus	15.51	kJ/mol	Joback Method
hvap	45.32	kJ/mol	Joback Method
ie	8.13	eV	NIST Webbook
log10ws	-4.57		Crippen Method
logp	4.907		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	521.88	K	Joback Method
tc	707.14	K	Joback Method
tf	154.54	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.23	J/mol×K	521.88	Joback Method
cpg	509.39	J/mol×K	552.76	Joback Method
cpg	528.59	J/mol×K	583.63	Joback Method
cpg	546.88	J/mol×K	614.51	Joback Method
cpg	564.28	J/mol×K	645.39	Joback Method
cpg	580.84	J/mol×K	676.26	Joback Method
cpg	596.59	J/mol×K	707.14	Joback Method

Sources

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=C7090882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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