(E)-3,4-Di-tert-butyl-3-hexene

Inchi: InChI=1S/C14H28/c1-9-11(13(3,4)5)12(10-2)14(6,7)8/h9-10H2,1-8H3/b12-11+
InchiKey: MVTUXXAVOOUGFH-VAWYXSNFSA-N
Formula: C14H28
SMILES: CCC(=C(CC)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 196.37
CAS: 75245-21-5

Physical Properties

Property code	Value	Unit	Source
gf	135.80	kJ/mol	Joback Method
hf	-168.30	kJ/mol	NIST Webbook
hfus	14.77	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	5.195		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
tb	517.18	K	Joback Method
tc	708.74	K	Joback Method
tf	219.38	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.46	J/mol×K	517.18	Joback Method
cpg	514.43	J/mol×K	549.11	Joback Method
cpg	534.19	J/mol×K	581.03	Joback Method
cpg	552.81	J/mol×K	612.96	Joback Method
cpg	570.35	J/mol×K	644.88	Joback Method
cpg	586.89	J/mol×K	676.81	Joback Method
cpg	602.50	J/mol×K	708.74	Joback Method

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=C75245215&Units=SI

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
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