di-t-Butylacetylene

Other names: 2,2,5,5-Tetramethyl-2-hexyne
(tert-C4H9)C«equiv»C(tert-C4H9)
Inchi: InChI=1S/C10H18/c1-9(2,3)7-8-10(4,5)6/h1-6H3
InchiKey: FXVDWKZNFZMSOU-UHFFFAOYSA-N
Formula: C10H18
SMILES: CC(C)(C)C#CC(C)(C)C
Mol. weight [g/mol]: 138.25
CAS: 17530-24-4

Physical Properties

Property code	Value	Unit	Source
gf	241.80	kJ/mol	Joback Method
hf	5.07	kJ/mol	Joback Method
hfus	9.95	kJ/mol	Joback Method
hvap	37.41	kJ/mol	Joback Method
ie	9.05 ± 0.01	eV	NIST Webbook
ie	8.98	eV	NIST Webbook
ie	9.19 ± 0.04	eV	NIST Webbook
log10ws	-3.32		Crippen Method
logp	3.082		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	430.74	K	Joback Method
tc	640.96	K	Joback Method
tf	292.60 ± 0.40	K	NIST Webbook
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.41	J/mol×K	430.74	Joback Method
cpg	310.03	J/mol×K	465.78	Joback Method
cpg	326.55	J/mol×K	500.81	Joback Method
cpg	342.02	J/mol×K	535.85	Joback Method

cpg	356.51	J/mol×K	570.88	Joback Method
cpg	370.08	J/mol×K	605.92	Joback Method
cpg	382.78	J/mol×K	640.96	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=C17530244&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
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