Diisopropenyldiacetylene

Inchi: InChI=1S/C10H10/c1-9(2)7-5-6-8-10(3)4/h1,3H2,2,4H3
InchiKey: FQFCHEWSAJOUPA-UHFFFAOYSA-N
Formula: C10H10
SMILES: C=C(C)C#CC#CC(=C)C
Mol. weight [g/mol]: 130.19
CAS: 5187-81-5

Physical Properties

Property code	Value	Unit	Source
chl	-5808.00 ± 2.00	kJ/mol	NIST Webbook
gf	597.50	kJ/mol	Joback Method
hf	494.10	kJ/mol	NIST Webbook
hfl	444.00 ± 2.00	kJ/mol	NIST Webbook
hfus	22.72	kJ/mol	Joback Method
hvap	50.20 ± 4.20	kJ/mol	NIST Webbook
log10ws	-3.31		Crippen Method
logp	2.145		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	439.32	K	Joback Method
tc	669.12	K	Joback Method
tf	383.22	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.58	J/mol×K	439.32	Joback Method
cpg	240.05	J/mol×K	477.62	Joback Method
cpg	251.82	J/mol×K	515.92	Joback Method
cpg	262.93	J/mol×K	554.22	Joback Method
cpg	273.42	J/mol×K	592.52	Joback Method
cpg	283.32	J/mol×K	630.82	Joback Method
cpg	292.66	J/mol×K	669.12	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=C5187815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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