Bullvalene

Inchi: InChI=1S/C10H10/c1-4-8-9-5-2-7(1)3-6-10(8)9/h1-10H
InchiKey: UKFBVTJTKMSPMI-UHFFFAOYSA-N
Formula: C10H10
SMILES: C1=CC2C3C=CC1C=CC23
Mol. weight [g/mol]: 130.19
CAS: 1005-51-2

Physical Properties

Property code	Value	Unit	Source
chs	-5626.50 ± 3.00	kJ/mol	NIST Webbook
gf	285.64	kJ/mol	Joback Method
hf	334.10 ± 3.30	kJ/mol	NIST Webbook
hfs	262.30 ± 3.30	kJ/mol	NIST Webbook
hfus	18.70	kJ/mol	Joback Method
hsub	71.80	kJ/mol	NIST Webbook
hsub	71.83	kJ/mol	NIST Webbook
hsub	71.80	kJ/mol	NIST Webbook
hvap	38.33	kJ/mol	Joback Method
ie	8.13	eV	NIST Webbook
ie	8.05	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.161		Crippen Method
mcvol	106.280	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
sg	337.10 ± 2.40	J/mol×K	NIST Webbook
sg	336.60 ± 1.00	J/mol×K	NIST Webbook
ss	174.66	J/mol×K	NIST Webbook
tb	445.50	K	Joback Method
tc	665.95	K	Joback Method
tf	250.80	K	Joback Method
tt	366.50 ± 0.10	K	NIST Webbook
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.75	J/mol×K	665.95	Joback Method
cpg	301.45	J/mol×K	629.21	Joback Method
cpg	289.17	J/mol×K	592.47	Joback Method
cpg	275.81	J/mol×K	555.73	Joback Method
cpg	261.26	J/mol×K	518.98	Joback Method
cpg	245.42	J/mol×K	482.24	Joback Method
cpg	228.17	J/mol×K	445.50	Joback Method
cps	190.38	J/mol×K	298.15	NIST Webbook
dvisc	0.0006665	Pa×s	348.15	Joback Method
dvisc	0.0009818	Pa×s	445.50	Joback Method
dvisc	0.0004440	Pa×s	283.25	Joback Method
dvisc	0.0003350	Pa×s	250.80	Joback Method
dvisc	0.0008805	Pa×s	413.05	Joback Method
dvisc	0.0007752	Pa×s	380.60	Joback Method
dvisc	0.0005555	Pa×s	315.70	Joback Method
hfust	15.25	kJ/mol	366.50	NIST Webbook
hfust	15.25	kJ/mol	366.50	NIST Webbook
hfust	15.25	kJ/mol	366.50	NIST Webbook
sfust	41.61	J/mol×K	366.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1005512&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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume