Azulene

Other names:	Azunamic
	Azusalen [as sodium sulfonate]
	BICYCLO(5.3.0)-DECA-2,4,6,8,10-PENTAENE
	Bicyclo(0.3.5)deca-1,3,5,7,9-pentaene
	Bicyclo(5.3.0)-1,3,5,7,9-decapentaene
	Bicyclo[5.3.0]decapentaene
	Cyclopentacycloheptene
	bicyclo[0.3.5]deca-1,3,5,7,9-pentaene
	bicyclo[5.3.0]deca-2,4,6,8,10-pentaene
Inchi:	InChI=1S/C10H8/c1-2-5-9-7-4-8-10(9)6-3-1/h1-8H
InchiKey:	CUFNKYGDVFVPHO-UHFFFAOYSA-N
Formula:	C10H8
SMILES:	c1ccc2cccc-2cc1
Mol. weight [g/mol]:	128.17
CAS:	275-51-4

Physical Properties

Property code	Value	Unit	Source
affp	927.60	kJ/mol	NIST Webbook
affp	925.20	kJ/mol	NIST Webbook
basg	896.00	kJ/mol	NIST Webbook
basg	896.60	kJ/mol	NIST Webbook
chl	-5293.00 ± 3.00	kJ/mol	NIST Webbook
chs	-5290.70	kJ/mol	NIST Webbook
ea	0.69 ± 0.04	eV	NIST Webbook
ea	0.79 ± 0.01	eV	NIST Webbook
ea	0.69 ± 0.10	eV	NIST Webbook
ea	0.46	eV	NIST Webbook
ea	0.52 ± 0.01	eV	NIST Webbook
ea	0.66 ± 0.01	eV	NIST Webbook
ea	0.80 ± 0.10	eV	NIST Webbook
ea	0.68 ± 0.04	eV	NIST Webbook
gf	252.38	kJ/mol	Joback Method
hf	280.00	kJ/mol	NIST Webbook
hf	308.00	kJ/mol	NIST Webbook
hfs	212.00	kJ/mol	NIST Webbook
hfus	12.72	kJ/mol	Joback Method

hsub	76.80 ± 0.20	kJ/mol	NIST Webbook
hsub	75.30	kJ/mol	NIST Webbook
hsub	82.90	kJ/mol	NIST Webbook
hsub	95.48 ± 0.42	kJ/mol	NIST Webbook
hsub	68.00	kJ/mol	NIST Webbook
hsub	95.40 ± 0.40	kJ/mol	NIST Webbook
hsub	72.70	kJ/mol	NIST Webbook
hvap	63.80 ± 0.20	kJ/mol	NIST Webbook
hvap	52.80	kJ/mol	NIST Webbook
ie	7.43 ± 0.04	eV	NIST Webbook
ie	7.42 ± 0.02	eV	NIST Webbook
ie	7.38 ± 0.03	eV	NIST Webbook
ie	7.32 ± 0.05	eV	NIST Webbook
ie	7.42	eV	NIST Webbook
ie	7.41 ± 0.05	eV	NIST Webbook
ie	7.43 ± 0.01	eV	NIST Webbook
ie	7.42 ± 0.05	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
ie	7.43 ± 0.01	eV	NIST Webbook
ie	7.44 ± 0.03	eV	NIST Webbook
ie	7.40	eV	NIST Webbook
log10ws	-3.49		Crippen Method
logp	2.791		Crippen Method
mcvol	108.540	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1329.70		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	223.74		NIST Webbook
rinpol	219.95		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	223.74		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1299.00		NIST Webbook
ripol	1736.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1736.00		NIST Webbook
tb	515.20	K	NIST Webbook
tc	711.47	K	Joback Method
tf	373.00 ± 2.00	K	NIST Webbook

tf	303.65 ± 1.00	K	NIST Webbook
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.18	J/mol×K	671.87	Joback Method
cpg	247.71	J/mol×K	592.67	Joback Method
cpg	236.07	J/mol×K	553.06	Joback Method
cpg	223.38	J/mol×K	513.46	Joback Method
cpg	209.58	J/mol×K	473.86	Joback Method
cpg	277.18	J/mol×K	711.47	Joback Method
cpg	258.39	J/mol×K	632.27	Joback Method
dvisc	0.0010984	Pa×s	296.96	Joback Method
dvisc	0.0007708	Pa×s	332.34	Joback Method
dvisc	0.0005791	Pa×s	367.72	Joback Method
dvisc	0.0004574	Pa×s	403.10	Joback Method
dvisc	0.0003754	Pa×s	438.48	Joback Method
dvisc	0.0017226	Pa×s	261.58	Joback Method
dvisc	0.0003173	Pa×s	473.86	Joback Method
hfust	17.53	kJ/mol	373.50	NIST Webbook
hsubt	78.40 ± 1.30	kJ/mol	304.50	NIST Webbook
hsubt	75.80	kJ/mol	273.00	NIST Webbook
hsubt	82.80	kJ/mol	331.00	NIST Webbook
hvapt	53.00	kJ/mol	442.00	NIST Webbook
hvapt	81.10	kJ/mol	298.15	Energetics and stability of azulene: From experimental thermochemistry to high-level quantum chemical calculations
hvapt	55.50	kJ/mol	398.00	NIST Webbook
hvapt	51.20	kJ/mol	488.00	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.51604e+01
Coeff. B	-6.61587e+03
Coeff. C	-1.23692e+02
Temperature range (K), min.	389.68
Temperature range (K), max.	457.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C275514&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Energetics and stability of azulene: From experimental thermochemistry to high-level quantum chemical calculations:	https://www.doi.org/10.1016/j.jct.2013.11.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume