Benz[e]indan

Other names:	2,3-dihydro-1H-benz[e]indene
	1h-Benz[e]indene, 2,3-dihydro-
Inchi:	InChI=1S/C13H12/c1-2-6-12-10(4-1)8-9-11-5-3-7-13(11)12/h1-2,4,6,8-9H,3,5,7H2
InchiKey:	HQYLCMKCKULOEV-UHFFFAOYSA-N
Formula:	C13H12
SMILES:	c1ccc2c3c(ccc2c1)CCC3
Mol. weight [g/mol]:	168.23
CAS:	4944-94-9

Physical Properties

Property code	Value	Unit	Source
gf	326.84	kJ/mol	Joback Method
hf	186.15	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	49.99	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.329		Crippen Method
mcvol	139.950	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	1578.00		NIST Webbook
tb	563.87	K	Joback Method
tc	808.97	K	Joback Method
tf	342.61	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.11	J/mol×K	563.87	Joback Method
cpg	393.87	J/mol×K	768.12	Joback Method
cpg	382.44	J/mol×K	727.27	Joback Method
cpg	370.08	J/mol×K	686.42	Joback Method
cpg	356.67	J/mol×K	645.57	Joback Method
cpg	342.05	J/mol×K	604.72	Joback Method

cpg	404.51	J/mol×K	808.97	Joback Method
dvisc	0.0005879	Pa×s	563.87	Joback Method
dvisc	0.0006573	Pa×s	526.99	Joback Method
dvisc	0.0007474	Pa×s	490.12	Joback Method
dvisc	0.0008678	Pa×s	453.24	Joback Method
dvisc	0.0010346	Pa×s	416.36	Joback Method
dvisc	0.0012763	Pa×s	379.49	Joback Method
dvisc	0.0016474	Pa×s	342.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	567.50 ± 0.50	K	101.00	NIST Webbook
tbrp	368.00 ± 5.00	K	0.01	NIST Webbook

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=C4944949&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume