Benzocycloheptene

Other names: Benzocycloheptene
Inchi: InChI=1S/C11H14/c1-2-6-10-8-4-5-9-11(10)7-3-1/h4-5,8-9H,1-3,6-7H2
InchiKey: HEOQXHNKRXRCTO-UHFFFAOYSA-N
Formula: C11H14
SMILES: c1ccc2c(c1)CCCCC2
Mol. weight [g/mol]: 146.23

Physical Properties

Property code	Value	Unit	Source
af	0.3213		Cheméo Relay (1.0)
gf	188.78	kJ/mol	Joback Method
hf	36.80	kJ/mol	Cheméo Relay (1.0)
hfus	10.76	kJ/mol	Joback Method
hvap	57.72	kJ/mol	Cheméo Relay (1.0)
ie	8.40 ± 0.02	eV	NIST Webbook
ie	8.44	eV	NIST Webbook
ie	9.10 ± 0.05	eV	NIST Webbook
log10ws	-3.96		Cheméo Relay (1.0)
logp	2.956		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	506.98	K	Cheméo Relay (1.0)
tc	733.02	K	Cheméo Relay (1.0)
tf	275.58	K	Cheméo Relay (1.0)
vc	0.474	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.58	J/mol×K	502.69	Joback Method
cpg	304.13	J/mol×K	542.28	Joback Method
cpg	321.38	J/mol×K	581.87	Joback Method
cpg	337.40	J/mol×K	621.46	Joback Method
cpg	352.26	J/mol×K	661.06	Joback Method

cpg	366.02	J/mol×K	700.65	Joback Method
cpg	378.75	J/mol×K	740.24	Joback Method
dvisc	0.0035581	Pa×s	267.81	Joback Method
dvisc	0.0017526	Pa×s	306.96	Joback Method
dvisc	0.0010133	Pa×s	346.10	Joback Method
dvisc	0.0006549	Pa×s	385.25	Joback Method
dvisc	0.0004587	Pa×s	424.40	Joback Method
dvisc	0.0003412	Pa×s	463.54	Joback Method
dvisc	0.0002658	Pa×s	502.69	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1075167&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
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