Benzocycloheptatriene

Other names: 3,4-Benzotropilidene
Inchi: InChI=1S/C11H10/c1-2-6-10-8-4-5-9-11(10)7-3-1/h1-6,8-9H,7H2
InchiKey: XHVULKQHRQZNMW-UHFFFAOYSA-N
Formula: C11H10
SMILES: C1=CCc2ccccc2C=C1
Mol. weight [g/mol]: 142.20
CAS: 264-09-5

Physical Properties

Property code	Value	Unit	Source
gf	248.70	kJ/mol	Joback Method
hf	151.07	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	44.17	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.812		Crippen Method
mcvol	122.630	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	220.30		NIST Webbook
rinpol	220.30		NIST Webbook
tb	501.01	K	Joback Method
tc	743.67	K	Joback Method
tf	269.33	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.65	J/mol×K	501.01	Joback Method
cpg	319.18	J/mol×K	703.23	Joback Method
cpg	307.83	J/mol×K	662.79	Joback Method
cpg	295.48	J/mol×K	622.34	Joback Method
cpg	282.05	J/mol×K	581.90	Joback Method
cpg	267.47	J/mol×K	541.45	Joback Method

cpg	329.61	J/mol×K	743.67	Joback Method
dvisc	0.0002615	Pa×s	501.01	Joback Method
dvisc	0.0003245	Pa×s	462.40	Joback Method
dvisc	0.0004189	Pa×s	423.78	Joback Method
dvisc	0.0005691	Pa×s	385.17	Joback Method
dvisc	0.0008278	Pa×s	346.56	Joback Method
dvisc	0.0013227	Pa×s	307.94	Joback Method
dvisc	0.0024177	Pa×s	269.33	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.80 ± 0.20	K	1.60	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=C264095&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