

Benz[a]ovalene

Inchi:	InChI=1S/C36H16/c1-2-4-24-23(3-1)25-14-13-19-8-11-21-15-20-10-7-17-5-6-18-9-12-22
InchiKey:	UEOJBRIZEMHGKR-UHFFFAOYSA-N
Formula:	C36H16
SMILES:	c1ccc2c(c1)c1ccc3ccc4cc5ccc6ccc7ccc8cc2c2c1c3c4c1c5c6c7c8c21
Mol. weight [g/mol]:	448.51
CAS:	75449-88-6

Physical Properties

Property code	Value	Unit	Source
gf	1315.68	kJ/mol	Joback Method
hf	1030.33	kJ/mol	Joback Method
hfus	64.62	kJ/mol	Joback Method
hvap	117.18	kJ/mol	Joback Method
log10ws	-16.59		Crippen Method
logp	10.408		Crippen Method
mcvol	321.240	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
tb	1245.88	K	Joback Method
tc	1533.31	K	Joback Method
tf	992.98	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.15	J/molxK	1245.88	Joback Method
cpg	1538.20	J/molxK	1485.41	Joback Method
cpg	1442.05	J/molxK	1437.50	Joback Method
cpg	1356.83	J/molxK	1389.60	Joback Method
cpg	1281.69	J/molxK	1341.69	Joback Method
cpg	1215.75	J/molxK	1293.79	Joback Method
cpg	1646.14	J/molxK	1533.31	Joback Method
dvisc	2.2745745	Paxs	1245.88	Joback Method
dvisc	2.1893823	Paxs	1203.73	Joback Method

dvisc	2.1015508	Paxs	1161.58	Joback Method
dvisc	2.0110325	Paxs	1119.43	Joback Method
dvisc	1.9177944	Paxs	1077.28	Joback Method
dvisc	1.8218221	Paxs	1035.13	Joback Method
dvisc	1.7231260	Paxs	992.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C75449886&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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