Dibenzo[a,e]cyclooctene

Inchi: InChI=1S/C16H12/c1-2-6-14-11-12-16-8-4-3-7-15(16)10-9-13(14)5-1/h1-12H/b10-9-,12-1
InchiKey: VGQWCQNHAMVTJY-YFDRDTFESA-N
Formula: C16H12
SMILES: C1=Cc2ccccc2C=Cc2ccccc21
Mol. weight [g/mol]: 204.27
CAS: 262-89-5

Physical Properties

Property code	Value	Unit	Source
gf	405.68	kJ/mol	Joback Method
hf	279.09	kJ/mol	Joback Method
hfus	21.91	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
log10ws	-4.93		Crippen Method
logp	4.341		Crippen Method
mcvol	169.320	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	642.80	K	Joback Method
tc	905.43	K	Joback Method
tf	368.14	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.52	J/mol×K	642.80	Joback Method
cpg	482.55	J/mol×K	861.65	Joback Method
cpg	470.95	J/mol×K	817.88	Joback Method
cpg	458.29	J/mol×K	774.11	Joback Method
cpg	444.42	J/mol×K	730.34	Joback Method
cpg	429.21	J/mol×K	686.57	Joback Method
cpg	493.25	J/mol×K	905.43	Joback Method
dvisc	0.0002560	Pa×s	642.80	Joback Method

dvisc	0.0003074	Pa×s	597.02	Joback Method
dvisc	0.0003805	Pa×s	551.25	Joback Method
dvisc	0.0004897	Pa×s	505.47	Joback Method
dvisc	0.0006626	Pa×s	459.69	Joback Method
dvisc	0.0009586	Pa×s	413.92	Joback Method
dvisc	0.0015202	Pa×s	368.14	Joback Method

Sources

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=C262895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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