10,11-Dihydro-5H-dibenzo(a,d)cycloheptene

Other names: 1,2:4,5-dibenzocycloheptane
10,11-dihydro-5H-dibenzo[a,d]cycloheptene
5H-Dibenzo[a,d]cycloheptene, 10,11-dihydro-
Inchi: InChI=1S/C15H14/c1-3-7-14-11-15-8-4-2-6-13(15)10-9-12(14)5-1/h1-8H,9-11H2
InchiKey: PJQCANLCUDUPRF-UHFFFAOYSA-N
Formula: C15H14
SMILES: c1ccc2c(c1)CCc1ccccc1C2
Mol. weight [g/mol]: 194.27
CAS: 833-48-7

Physical Properties

Property code	Value	Unit	Source
gf	349.44	kJ/mol	Joback Method
hf	190.33	kJ/mol	Joback Method
hfus	103.60	kJ/mol	Experimental and computational study on the energetics of 10,11-dihydro-5H-dibenzo[a,d]cyclohepten (dibenzosuberane)
hvap	55.08	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.376		Crippen Method
mcvol	163.830	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
tb	617.33	K	Joback Method
tc	871.81	K	Joback Method
tf	358.87	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.56	J/mol×K	617.33	Joback Method
cpg	422.35	J/mol×K	659.74	Joback Method
cpg	438.66	J/mol×K	702.16	Joback Method

cpg	453.64	J/mol×K	744.57	Joback Method
cpg	467.41	J/mol×K	786.98	Joback Method
cpg	480.11	J/mol×K	829.39	Joback Method
cpg	491.88	J/mol×K	871.81	Joback Method
dvisc	0.0017632	Pa×s	358.87	Joback Method
dvisc	0.0011542	Pa×s	401.95	Joback Method
dvisc	0.0008201	Pa×s	445.02	Joback Method
dvisc	0.0006189	Pa×s	488.10	Joback Method
dvisc	0.0004889	Pa×s	531.18	Joback Method
dvisc	0.0004002	Pa×s	574.25	Joback Method
dvisc	0.0003368	Pa×s	617.33	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.70	K	0.30	NIST Webbook

Sources

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

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

Experimental and computational study on the energetics of 10,11-dihydro-5H-dibenzo[a,d]cycloheptene (dibenzosuberane): https://www.doi.org/10.1016/j.jct.2010.10.009

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=C833487&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume