

5,6,6a,7,8,12b,12c-Octahydrodibenzo[a,i]biphenyl

Inchi: InChI=1S/C20H20/c1-3-7-15-13(5-1)9-11-17-18-12-10-14-6-2-4-8-16(14)20(18)19(15)17
InchiKey: LKMAMCWAHCZBAI-UHFFFAOYSA-N
Formula: C20H20
SMILES: c1ccc2c(c1)CCC1C3CCc4ccccc4C3C21
Mol. weight [g/mol]: 260.37
CAS: 42182-84-3

Physical Properties

Property code	Value	Unit	Source
chs	-10808.70 ± 1.50	kJ/mol	NIST Webbook
chs	-10808.70 ± 1.50	kJ/mol	NIST Webbook
gf	509.72	kJ/mol	Joback Method
hf	198.21	kJ/mol	Joback Method
hfs	80.10 ± 1.80	kJ/mol	NIST Webbook
hfs	80.10 ± 1.80	kJ/mol	NIST Webbook
hfus	32.44	kJ/mol	Joback Method
hvap	65.25	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.692		Crippen Method
mcvol	212.560	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
tb	731.60	K	Joback Method
tc	984.10	K	Joback Method
tf	446.14	K	Joback Method
vc	0.818	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.58	J/mol×K	731.60	Joback Method
cpg	661.98	J/mol×K	773.68	Joback Method
cpg	680.89	J/mol×K	815.77	Joback Method
cpg	698.56	J/mol×K	857.85	Joback Method
cpg	715.21	J/mol×K	899.93	Joback Method

cpg	731.08	J/mol×K	942.02	Joback Method
cpg	746.41	J/mol×K	984.10	Joback Method
cpl	333.40	J/mol×K	298.15	NIST Webbook
dvisc	0.0042492	Paxs	446.14	Joback Method
dvisc	0.0041143	Paxs	493.72	Joback Method
dvisc	0.0040063	Paxs	541.29	Joback Method
dvisc	0.0039180	Paxs	588.87	Joback Method
dvisc	0.0038444	Paxs	636.45	Joback Method
dvisc	0.0037821	Paxs	684.02	Joback Method
dvisc	0.0037288	Paxs	731.60	Joback Method

Sources

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=C42182843&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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