

6b,8a-Dihydrocyclobut[a]acenaphthylene

Inchi:	InChI=1S/C14H10/c1-3-9-4-2-6-13-11-8-7-10(11)12(5-1)14(9)13/h1-8,10-11H
InchiKey:	MKRSL SRLZZVPKE-UHFFFAOYSA-N
Formula:	C14H10
SMILES:	C1=CC2c3cccc4cccc(c34)C12
Mol. weight [g/mol]:	178.23
CAS:	30736-79-9

Physical Properties

Property code	Value	Unit	Source
gf	442.46	kJ/mol	Joback Method
hf	288.07	kJ/mol	Joback Method
hfus	23.99	kJ/mol	Joback Method
hvap	51.77	kJ/mol	Joback Method
ie	7.72	eV	NIST Webbook
log10ws	-4.45		Crippen Method
logp	3.590		Crippen Method
mcvol	138.880	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	579.44	K	Joback Method
tc	822.62	K	Joback Method
tf	375.38	K	Joback Method
vc	0.549	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.08	J/molxK	579.44	Joback Method
cpg	353.67	J/molxK	619.97	Joback Method
cpg	366.91	J/molxK	660.50	Joback Method
cpg	379.00	J/molxK	701.03	Joback Method
cpg	390.13	J/molxK	741.56	Joback Method
cpg	400.48	J/molxK	782.09	Joback Method
cpg	410.24	J/molxK	822.62	Joback Method
dvisc	0.0019051	Paxs	375.38	Joback Method

dvisc	0.0020324	Paxs	409.39	Joback Method
dvisc	0.0021467	Paxs	443.40	Joback Method
dvisc	0.0022499	Paxs	477.41	Joback Method
dvisc	0.0023433	Paxs	511.42	Joback Method
dvisc	0.0024283	Paxs	545.43	Joback Method
dvisc	0.0025059	Paxs	579.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30736799&Units=SI
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

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

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