

Cyclobuta[1,2-a:3,4-a']diacenaphthylene, 6b,6c,12b,12c-tetrahydro- (6b«alpha»,6c«beta»,12b«beta»,12c«alpha»)-

InChI: InChI=1S/C24H16/c1-5-16-8-2-10-16-19(13)15(9,11)21-22(16)14-18-12-4-8-14-7-3-11-17
InChIKey: TVMWOWUBPJYVYIG-NVPYSNMXSA-N
Formula: C24H16
SMILES: c1cc2c3c(cccc3c1)C1C2C2c3cccc4cccc(c34)C12
Mol. weight [g/mol]: 304.38
CAS: 14620-98-5

Physical Properties

Property code	Value	Unit	Source
gf	785.84	kJ/mol	Joback Method
hf	499.49	kJ/mol	Joback Method
hfus	44.46	kJ/mol	Joback Method
hvap	78.07	kJ/mol	Joback Method
ie	7.48	eV	NIST Webbook
log10ws	-7.81		Crippen Method
logp	6.068		Crippen Method
mccvol	230.000	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
tb	853.96	K	Joback Method
tc	1111.91	K	Joback Method
tf	595.74	K	Joback Method
vc	0.917	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.35	J/molxK	853.96	Joback Method
cpg	723.79	J/molxK	896.95	Joback Method
cpg	740.18	J/molxK	939.94	Joback Method
cpg	756.90	J/molxK	982.94	Joback Method
cpg	774.33	J/molxK	1025.93	Joback Method
cpg	792.87	J/molxK	1068.92	Joback Method
cpg	812.89	J/molxK	1111.91	Joback Method
dvisc	0.0358504	Paxs	595.74	Joback Method

dvisc	0.0402571	Paxs	638.78	Joback Method
dvisc	0.0445486	Paxs	681.81	Joback Method
dvisc	0.0487082	Paxs	724.85	Joback Method
dvisc	0.0527260	Paxs	767.89	Joback Method
dvisc	0.0565971	Paxs	810.92	Joback Method
dvisc	0.0603200	Paxs	853.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14620985&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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