

Pentacyclo[13.3.2.2^{6,10}.1^{3,18}

Other names:	Pentacyclo[13.3.2.2
Inchi:	InChI=1S/C24H20/c1-2-18-7-11-23-15-20(16-24(23)12-8-18)4-3-19-13-21-9-5-17(1)6-10
InchiKey:	SOJCCVPXRNRQYQH-UHFFFAOYSA-N
Formula:	C24H20
SMILES:	c1cc2cc3cc-2ccc1CCc1ccc2cc(cc-2cc1)CC3
Mol. weight [g/mol]:	308.42
CAS:	73608-52-3

Physical Properties

Property code	Value	Unit	Source
gf	607.16	kJ/mol	Joback Method
hf	357.61	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	79.89	kJ/mol	Joback Method
ie	6.60	eV	NIST Webbook
log10ws	-8.59		Crippen Method
logp	5.780		Crippen Method
mcvol	251.720	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
tb	875.44	K	Joback Method
tc	1145.80	K	Joback Method
tf	547.22	K	Joback Method
vc	0.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.43	J/molxK	875.44	Joback Method
cpg	772.92	J/molxK	920.50	Joback Method
cpg	789.45	J/molxK	965.56	Joback Method
cpg	805.27	J/molxK	1010.62	Joback Method
cpg	820.66	J/molxK	1055.68	Joback Method
cpg	835.89	J/molxK	1100.74	Joback Method
cpg	851.22	J/molxK	1145.80	Joback Method

dvisc	0.0014536	Paxs	547.22	Joback Method
dvisc	0.0010812	Paxs	601.92	Joback Method
dvisc	0.0008448	Paxs	656.63	Joback Method
dvisc	0.0006857	Paxs	711.33	Joback Method
dvisc	0.0005733	Paxs	766.03	Joback Method
dvisc	0.0004910	Paxs	820.74	Joback Method
dvisc	0.0004287	Paxs	875.44	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=C73608523&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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