

Pentacyclo[10.4.4.4^{4,9}.0^{6,23}

Other names:	Pentacyclo[10.4.4.4 ^{4,9} .0 ^{6,22} .0 ^{15,19}]tetracosa-4, Pentacyclo[10.4.4.4
Inchi:	InChI=1S/C24H20/c1-2-18-6-10-24-16-20(8-12-23(24)14-18)4-3-19-7-11-21-13-17(1)5-9
InchiKey:	YOFPSRWBZCXYAY-UHFFFAOYSA-N
Formula:	C24H20
SMILES:	c1cc2cc3ccc2cc1CCc1ccc2cc(ccc2c1)CC3
Mol. weight [g/mol]:	308.42
CAS:	73608-51-2

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	7.52	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
log10ws	-8.16		Crippen Method
logp	5.877		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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.43	J/mol×K	875.44	Joback Method
cpg	772.92	J/mol×K	920.50	Joback Method
cpg	789.45	J/mol×K	965.56	Joback Method
cpg	805.27	J/mol×K	1010.62	Joback Method
cpg	820.66	J/mol×K	1055.68	Joback Method

cpg	835.89	J/mol×K	1100.74	Joback Method
cpg	851.22	J/mol×K	1145.80	Joback Method
dvisc	0.0014536	Pa×s	547.22	Joback Method
dvisc	0.0010812	Pa×s	601.92	Joback Method
dvisc	0.0008448	Pa×s	656.63	Joback Method
dvisc	0.0006857	Pa×s	711.33	Joback Method
dvisc	0.0005733	Pa×s	766.03	Joback Method
dvisc	0.0004910	Pa×s	820.74	Joback Method
dvisc	0.0004287	Pa×s	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=C73608512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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