

Spiro[4.5]decane

Other names:	Spiro[4.5]decane Spiro(4,5)decane
Inchi:	InChI=1S/C10H18/c1-2-6-10(7-3-1)8-4-5-9-10/h1-9H2
InchiKey:	CTDQAGUNKPRERK-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	C1CCC2(CC1)CCCC2
Mol. weight [g/mol]:	138.25
CAS:	176-63-6

Physical Properties

Property code	Value	Unit	Source
chl	-6307.50 ± 2.00	kJ/mol	NIST Webbook
chl	-6307.00 ± 1.00	kJ/mol	NIST Webbook
gf	108.64	kJ/mol	Joback Method
hf	-145.10 ± 2.20	kJ/mol	NIST Webbook
hfl	-200.00 ± 1.00	kJ/mol	NIST Webbook
hfus	2.16	kJ/mol	Joback Method
hvap	54.80	kJ/mol	NIST Webbook
hvap	54.92 ± 0.09	kJ/mol	NIST Webbook
log10ws	-3.56		Crippen Method
logp	3.511		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	458.00 ± 3.00	K	NIST Webbook
tc	696.17	K	Joback Method
tf	252.40	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.02	J/mol×K	463.67	Joback Method
cpg	309.42	J/mol×K	502.42	Joback Method
cpg	330.05	J/mol×K	541.17	Joback Method

cpg	349.09	J/mol×K	579.92	Joback Method
cpg	366.72	J/mol×K	618.67	Joback Method
cpg	383.11	J/mol×K	657.42	Joback Method
cpg	398.44	J/mol×K	696.17	Joback Method
hvapt	44.00	kJ/mol	368.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C176636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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