

Spiro[5.5]undecane

Other names:	Spiro(5,5)undecane
Inchi:	InChI=1S/C11H20/c1-3-7-11(8-4-1)9-5-2-6-10-11/h1-10H2
InchiKey:	NECLQTPQJZSWOE-UHFFFAOYSA-N
Formula:	C11H20
SMILES:	C1CCC2(CC1)CCCCC2
Mol. weight [g/mol]:	152.28
CAS:	180-43-8

Physical Properties

Property code	Value	Unit	Source
chl	-6942.40 ± 2.80	kJ/mol	NIST Webbook
chl	-6939.00 ± 2.00	kJ/mol	NIST Webbook
gf	104.96	kJ/mol	Joback Method
hf	-191.80	kJ/mol	NIST Webbook
hf	-188.30 ± 3.10	kJ/mol	NIST Webbook
hfl	-248.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-244.50 ± 3.00	kJ/mol	NIST Webbook
hfus	2.65	kJ/mol	Joback Method
hsub	63.60 ± 0.80	kJ/mol	NIST Webbook
hvap	56.20	kJ/mol	NIST Webbook
hvap	56.10	kJ/mol	NIST Webbook
hvap	56.10 ± 0.10	kJ/mol	NIST Webbook
log10ws	-3.97		Crippen Method
logp	3.901		Crippen Method
mcvol	144.130	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
tb	490.82	K	Joback Method
tc	728.55	K	Joback Method
tf	248.65 ± 0.50	K	NIST Webbook
tf	248.70 ± 0.50	K	NIST Webbook
tf	248.70 ± 0.60	K	NIST Webbook
vc	0.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.74	J/mol×K	490.82	Joback Method
cpg	358.84	J/mol×K	530.44	Joback Method
cpg	381.11	J/mol×K	570.06	Joback Method
cpg	401.73	J/mol×K	609.68	Joback Method
cpg	420.89	J/mol×K	649.31	Joback Method
cpg	438.77	J/mol×K	688.93	Joback Method
cpg	455.56	J/mol×K	728.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.55909e+01
Coeff. B	-3.44213e+03
Coeff. C	-1.69238e+02
Temperature range (K), min.	369.00
Temperature range (K), max.	504.09

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=C180438&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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