Spiro[5.6]dodecane

Other names: Spiro(5,6)dodecane
Inchi: InChI=1S/C12H22/c1-2-5-9-12(8-4-1)10-6-3-7-11-12/h1-11H2
InchiKey: ZDNANLAHKKNCTC-UHFFFAOYSA-N
Formula: C12H22
SMILES: C1CCCC2(CC1)CCCCC2
Mol. weight [g/mol]: 166.30
CAS: 181-15-7

Physical Properties

Property code	Value	Unit	Source
gf	101.28	kJ/mol	Joback Method
hf	-146.79	kJ/mol	Joback Method
hfus	3.14	kJ/mol	Joback Method
hvap	42.32	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.291		Crippen Method
mcvol	158.220	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	517.97	K	Joback Method
tc	760.42	K	Joback Method
tf	267.90	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.02	J/mol×K	517.97	Joback Method
cpg	410.75	J/mol×K	558.38	Joback Method
cpg	434.58	J/mol×K	598.79	Joback Method
cpg	456.72	J/mol×K	639.20	Joback Method
cpg	477.33	J/mol×K	679.60	Joback Method
cpg	496.62	J/mol×K	720.01	Joback Method
cpg	514.77	J/mol×K	760.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.81411e+01
Coeff. B	-1.18250e+04
Temperature range (K), min.	424.54
Temperature range (K), max.	517.97

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=C181157&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
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