Spiro[4.5]decane, 7-hexadecyl-

Other names: 7-Hexadecylspiro[4.5]decane
7-n-Hexadecylspiro[4.5]decane
Inchi: InChI=1S/C26H50/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-25-20-18-23-26(24-25)21-1
InchiKey: BNDDTWKJQMCKBA-UHFFFAOYSA-N
Formula: C26H50
SMILES: CCCCCCCCCCCCCCCCC1CCCC2(CCCC2)C1
Mol. weight [g/mol]: 362.68
CAS: 2307-06-4

Physical Properties

Property code	Value	Unit	Source
chl	-16786.50 ± 2.20	kJ/mol	NIST Webbook
gf	235.65	kJ/mol	Joback Method
hf	-443.77	kJ/mol	Joback Method
hfl	-590.40 ± 2.40	kJ/mol	NIST Webbook
hfus	44.67	kJ/mol	Joback Method
hvap	72.83	kJ/mol	Joback Method
log10ws	-10.01		Crippen Method
logp	9.608		Crippen Method
mcvol	355.480	ml/mol	McGowan Method
pc	913.29	kPa	Joback Method
tb	825.08	K	Joback Method
tc	1019.91	K	Joback Method
tf	428.48	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.12	J/mol×K	825.08	Joback Method
cpg	1230.04	J/mol×K	857.55	Joback Method
cpg	1255.03	J/mol×K	890.02	Joback Method
cpg	1279.23	J/mol×K	922.49	Joback Method
cpg	1302.78	J/mol×K	954.97	Joback Method

cpg	1325.81	J/mol×K	987.44	Joback Method
cpg	1348.47	J/mol×K	1019.91	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.19832e+01
Coeff. B	-5.17298e+03
Temperature range (K), min.	442.30
Temperature range (K), max.	775.36

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=C2307064&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

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
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