Hexacyclopropylethane

Inchi: InChI=1S/C20H30/c1-2-13(1)19(14-3-4-14,15-5-6-15)20(16-7-8-16,17-9-10-17)18-11-12-
InchiKey: SKEXUOOOMGGNIA-UHFFFAOYSA-N
Formula: C20H30
SMILES: C1CC1C(C1CC1)(C1CC1)C(C1CC1)(C1CC1)C1CC1
Mol. weight [g/mol]: 270.45
CAS: 26902-55-6

Physical Properties

Property code	Value	Unit	Source
gf	487.70	kJ/mol	Joback Method
hf	466.50	kJ/mol	NIST Webbook
hfs	357.50 ± 3.90	kJ/mol	NIST Webbook
hfus	21.54	kJ/mol	Joback Method
hsub	109.00	kJ/mol	NIST Webbook
hsub	109.00 ± 2.00	kJ/mol	NIST Webbook
hvap	85.80 ± 0.20	kJ/mol	NIST Webbook
log10ws	-5.63		Crippen Method
logp	5.419		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
tb	690.98	K	Joback Method
tc	932.89	K	Joback Method
tf	427.64	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.12	J/mol×K	690.98	Joback Method
cpg	791.16	J/mol×K	731.30	Joback Method
cpg	815.23	J/mol×K	771.62	Joback Method
cpg	837.69	J/mol×K	811.94	Joback Method
cpg	858.94	J/mol×K	852.26	Joback Method
cpg	879.35	J/mol×K	892.57	Joback Method

cpg	899.30	J/mol×K	932.89	Joback Method
cps	396.10	J/mol×K	298.15	NIST Webbook
dvisc	0.0175841	Pa×s	427.64	Joback Method
dvisc	0.0192687	Pa×s	471.53	Joback Method
dvisc	0.0207883	Pa×s	515.42	Joback Method
dvisc	0.0221621	Pa×s	559.31	Joback Method
dvisc	0.0234076	Pa×s	603.20	Joback Method
dvisc	0.0245405	Pa×s	647.09	Joback Method
dvisc	0.0255742	Pa×s	690.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C26902556&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume