1,8-Paracyclophane

Inchi: InChI=1S/C21H26/c1-2-4-6-8-19-11-15-21(16-12-19)17-20-13-9-18(10-14-20)7-5-3-1/h9-
InchiKey: DMCPGMNUZQZGNM-UHFFFAOYSA-N
Formula: C21H26
SMILES: c1cc2ccc1CCCCCCCCc1ccc(cc1)C2
Mol. weight [g/mol]: 278.43
CAS: 6169-94-4

Physical Properties

Property code	Value	Unit	Source
chs	-11898.00 ± 7.10	kJ/mol	NIST Webbook
gf	327.36	kJ/mol	Joback Method
hf	29.00 ± 9.20	kJ/mol	NIST Webbook
hfs	-82.00 ± 7.10	kJ/mol	NIST Webbook
hfus	21.91	kJ/mol	Joback Method
hsub	111.00	kJ/mol	NIST Webbook
hsub	111.00 ± 2.00	kJ/mol	NIST Webbook
hsub	110.90 ± 2.10	kJ/mol	NIST Webbook
hvap	69.47	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.717		Crippen Method
mcvol	248.370	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
tb	780.23	K	Joback Method
tc	1048.60	K	Joback Method
tf	405.37	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.68	J/mol×K	1048.60	Joback Method
cpg	844.58	J/mol×K	1003.87	Joback Method
cpg	829.57	J/mol×K	959.14	Joback Method
cpg	812.55	J/mol×K	914.42	Joback Method

cpg	793.41	J/mol×K	869.69	Joback Method
cpg	772.05	J/mol×K	824.96	Joback Method
cpg	748.39	J/mol×K	780.23	Joback Method
dvisc	0.0012679	Pa×s	405.37	Joback Method
dvisc	0.0000265	Pa×s	780.23	Joback Method
dvisc	0.0000381	Pa×s	717.75	Joback Method
dvisc	0.0000588	Pa×s	655.28	Joback Method
dvisc	0.0000994	Pa×s	592.80	Joback Method
dvisc	0.0001901	Pa×s	530.32	Joback Method
dvisc	0.0004326	Pa×s	467.85	Joback Method
hsubt	105.00 ± 1.30	kJ/mol	365.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67687e+01
Coeff. B	-7.64741e+03
Temperature range (K), min.	464.01
Temperature range (K), max.	667.47

Sources

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

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=C6169944&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas 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
hsubt:	Enthalpy of sublimation at a given temperature
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