Ovalene

Inchi: InChI=1S/C32H14/c1-2-16-6-10-20-14-22-12-8-18-4-3-17-7-11-21-13-19-9-5-15(1)23-24(
InchiKey: LSQODMMMSXHVCN-UHFFFAOYSA-N
Formula: C32H14
SMILES: c1cc2ccc3cc4ccc5ccc6ccc7cc8ccc1c1c2c3c2c4c5c6c7c2c81
Mol. weight [g/mol]: 398.45
CAS: 190-26-1

Physical Properties

Property code	Value	Unit	Source
gf	1184.98	kJ/mol	Joback Method
hf	933.29	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	105.98	kJ/mol	Joback Method
ie	6.71	eV	NIST Webbook
ie	6.86 ± 0.01	eV	NIST Webbook
ie	7.20 ± 0.10	eV	NIST Webbook
ie	7.01	eV	NIST Webbook
ie	6.71	eV	NIST Webbook
log10ws	-14.79		Crippen Method
logp	9.254		Crippen Method
mcvol	284.340	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
tb	1130.40	K	Joback Method
tc	1404.85	K	Joback Method
tf	770.10 ± 0.60	K	NIST Webbook
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.23	J/mol×K	1130.40	Joback Method
cpg	1168.18	J/mol×K	1359.11	Joback Method
cpg	1106.73	J/mol×K	1313.37	Joback Method
cpg	1052.70	J/mol×K	1267.63	Joback Method

cpg	1005.41	J/mol×K	1221.88	Joback Method
cpg	964.14	J/mol×K	1176.14	Joback Method
cpg	1237.74	J/mol×K	1404.85	Joback Method
dvisc	0.9049273	Pa×s	940.63	Joback Method
dvisc	0.9581490	Pa×s	978.59	Joback Method
dvisc	1.0101807	Pa×s	1016.54	Joback Method
dvisc	1.0609916	Pa×s	1054.49	Joback Method
dvisc	1.1105648	Pa×s	1092.45	Joback Method
dvisc	0.8505645	Pa×s	902.68	Joback Method
dvisc	1.1588952	Pa×s	1130.40	Joback Method
hfust	17.40	kJ/mol	770.10	NIST Webbook
hfust	8.08	kJ/mol	729.00	NIST Webbook
hfust	17.40	kJ/mol	770.10	NIST Webbook
hsubt	211.70 ± 7.90	kJ/mol	600.00	NIST Webbook
sfust	22.59	J/mol×K	770.10	NIST Webbook
sfust	11.08	J/mol×K	729.00	NIST Webbook

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=C190261&Units=SI
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
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume