

Octahelicene

Inchi: InChI=1S/C34H20/c1-2-6-22-10-26-14-30-18-34-20-32-16-28-12-24-8-4-3-7-23(24)11-27
InchiKey: PFTXKXWAXWAZBP-UHFFFAOYSA-N
Formula: C34H20
SMILES: c1ccc2cc3cc4cc5cc6cc7cc8ccccc8cc7cc6cc5cc4cc3cc2c1
Mol. weight [g/mol]: 428.52

Physical Properties

Property code	Value	Unit	Source
gf	1036.58	kJ/mol	Joback Method
hf	760.11	kJ/mol	Joback Method
hfus	54.66	kJ/mol	Joback Method
hvap	109.01	kJ/mol	Joback Method
log10ws	-14.10		Crippen Method
logp	9.759		Crippen Method
mcvol	329.940	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	3950.00		NIST Webbook
rinpol	3950.00		NIST Webbook
rinpol	3958.00		NIST Webbook
rinpol	3950.00		NIST Webbook
rinpol	3958.00		NIST Webbook
tb	1166.74	K	Joback Method
tc	1453.32	K	Joback Method
tf	803.38	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.53	J/molxK	1166.74	Joback Method
cpg	1259.98	J/molxK	1405.55	Joback Method
cpg	1216.88	J/molxK	1357.79	Joback Method
cpg	1178.32	J/molxK	1310.03	Joback Method
cpg	1143.78	J/molxK	1262.27	Joback Method

cpg	1112.70	J/molxK	1214.50	Joback Method
cpg	1308.19	J/molxK	1453.32	Joback Method
dvisc	0.0044102	Paxs	1166.74	Joback Method
dvisc	0.0046557	Paxs	1106.18	Joback Method
dvisc	0.0049459	Paxs	1045.62	Joback Method
dvisc	0.0052934	Paxs	985.06	Joback Method
dvisc	0.0057159	Paxs	924.50	Joback Method
dvisc	0.0062390	Paxs	863.94	Joback Method
dvisc	0.0069004	Paxs	803.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R525332&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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