

Nonahelicene

Inchi:	InChI=1S/C38H22/c1-2-6-24-10-28-14-32-18-36-22-38-20-34-16-30-12-26-8-4-3-7-25(26
InchiKey:	UIFXPOUSHBMMEG-UHFFFAOYSA-N
Formula:	C38H22
SMILES:	c1ccc2cc3cc4cc5cc6cc7cc8cc9ccccc9cc8cc7cc6cc5cc4cc3cc2c1
Mol. weight [g/mol]:	478.58

Physical Properties

Property code	Value	Unit	Source
gf	1167.28	kJ/mol	Joback Method
hf	857.15	kJ/mol	Joback Method
hfus	61.65	kJ/mol	Joback Method
hvap	120.21	kJ/mol	Joback Method
log10ws	-15.91		Crippen Method
logp	10.912		Crippen Method
mcvol	366.840	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	4260.00		NIST Webbook
rinpol	4265.00		NIST Webbook
rinpol	4260.00		NIST Webbook
rinpol	4260.00		NIST Webbook
rinpol	4265.00		NIST Webbook
tb	1282.22	K	Joback Method
tc	1580.19	K	Joback Method
tf	893.68	K	Joback Method
vc	1.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.69	J/molxK	1282.22	Joback Method
cpg	1332.23	J/molxK	1331.88	Joback Method
cpg	1379.99	J/molxK	1381.54	Joback Method
cpg	1433.68	J/molxK	1431.21	Joback Method
cpg	1493.99	J/molxK	1480.87	Joback Method

cpg	1561.60	J/molxK	1530.53	Joback Method
cpg	1637.22	J/molxK	1580.19	Joback Method
dvisc	0.0104640	Paxs	893.68	Joback Method
dvisc	0.0095691	Paxs	958.44	Joback Method
dvisc	0.0088502	Paxs	1023.19	Joback Method
dvisc	0.0082618	Paxs	1087.95	Joback Method
dvisc	0.0077724	Paxs	1152.71	Joback Method
dvisc	0.0073596	Paxs	1217.46	Joback Method
dvisc	0.0070073	Paxs	1282.22	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R525327&Units=SI

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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