Nonacene

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
CAS: 258-36-6

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
tb	1282.22	K	Joback Method
tc	1580.19	K	Joback Method
tf	893.68	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.69	J/mol×K	1282.22	Joback Method
cpg	1332.23	J/mol×K	1331.88	Joback Method
cpg	1379.99	J/mol×K	1381.54	Joback Method
cpg	1433.68	J/mol×K	1431.21	Joback Method
cpg	1493.99	J/mol×K	1480.87	Joback Method
cpg	1561.60	J/mol×K	1530.53	Joback Method
cpg	1637.22	J/mol×K	1580.19	Joback Method
dvisc	0.0104640	Pa×s	893.68	Joback Method
dvisc	0.0095691	Pa×s	958.44	Joback Method

dvisc	0.0088502	Pa×s	1023.19	Joback Method
dvisc	0.0082618	Pa×s	1087.95	Joback Method
dvisc	0.0077724	Pa×s	1152.71	Joback Method
dvisc	0.0073596	Pa×s	1217.46	Joback Method
dvisc	0.0070073	Pa×s	1282.22	Joback Method

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=C258366&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
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