1-Phenyl-2-(2-hexahelicenyl)ethylene, trans

Inchi: InChI=1S/C34H22/c1-2-7-23(8-3-1)13-14-24-11-6-12-27-17-30-20-31-18-28-15-25-9-4-5-
InchiKey: AEXQMPNELWCXDO-BUHFOSPRSA-N
Formula: C34H22
SMILES: C(=Cc1cccc2cc3cc4cc5cc6ccccc6cc5cc4cc3cc12)c1ccccc1
Mol. weight [g/mol]: 430.54

Physical Properties

Property code	Value	Unit	Source
gf	1025.54	kJ/mol	Joback Method
hf	743.19	kJ/mol	Joback Method
hfus	55.25	kJ/mol	Joback Method
hvap	107.30	kJ/mol	Joback Method
log10ws	-13.10		Crippen Method
logp	9.623		Crippen Method
mcvol	340.800	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinpol	4180.00		NIST Webbook
rinpol	4180.00		NIST Webbook
rinpol	4180.00		NIST Webbook
rinpol	4180.00		NIST Webbook
tb	1154.64	K	Joback Method
tc	1439.45	K	Joback Method
tf	746.80	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1110.24	J/mol×K	1154.64	Joback Method
cpg	1262.28	J/mol×K	1391.98	Joback Method
cpg	1225.68	J/mol×K	1344.51	Joback Method
cpg	1192.68	J/mol×K	1297.04	Joback Method
cpg	1162.76	J/mol×K	1249.58	Joback Method
cpg	1135.45	J/mol×K	1202.11	Joback Method

cpg	1302.96	J/mol×K	1439.45	Joback Method
dvisc	0.0007860	Pa×s	1154.64	Joback Method
dvisc	0.0008670	Pa×s	1086.67	Joback Method
dvisc	0.0009689	Pa×s	1018.69	Joback Method
dvisc	0.0011003	Pa×s	950.72	Joback Method
dvisc	0.0012741	Pa×s	882.75	Joback Method
dvisc	0.0015119	Pa×s	814.77	Joback Method
dvisc	0.0018508	Pa×s	746.80	Joback Method

Sources

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=R525258&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.