Pentacyclo[3.3.3.02,4.06,8.09.11]undecane, stereoisomer

Other names: Pentacyclo[3.3.3.0

Inchi: InChI=1S/C11H14/c1-4-5(1)11-7-2-6(7)10(4)8-3-9(8)11/h4-11H,1-3H2

InchiKey: TZRQBQARGUABOE-UHFFFAOYSA-N

Formula: C11H14

SMILES: C1C2C1C1C3CC3C2C2CC21

Mol. weight [g/mol]: 146.23

Physical Properties

Property code	Value	Unit	Source
hf	240.03	kJ/mol	Cheméo Relay (1.0)
hfus	26.53	kJ/mol	Joback Method
hvap	50.97	kJ/mol	Cheméo Relay (1.0)
ie	8.60	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
logp	2.154		Crippen Method
mcvol	111.550	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.40	J/mol×K	453.69	Joback Method
cpg	311.69	J/mol×K	487.53	Joback Method
cpg	330.28	J/mol×K	521.36	Joback Method
cpg	347.32	J/mol×K	555.20	Joback Method
cpg	362.97	J/mol×K	589.04	Joback Method
cpg	377.36	J/mol×K	622.87	Joback Method
cpg	390.67	J/mol×K	656.71	Joback Method
dvisc	0.0003758	Pa×s	304.79	Joback Method
dvisc	0.0007560	Pa×s	329.61	Joback Method
dvisc	0.0013791	Pa×s	354.42	Joback Method
dvisc	0.0023253	Pa×s	379.24	Joback Method
dvisc	0.0036770	Pa×s	404.06	Joback Method
dvisc	0.0055142	Pa×s	428.87	Joback Method
dvisc	0.0079106	Pa×s	453.69	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70469895&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume