Tricyclo[4.3.1.12,5]undec-3-ene, (1α,2β,5β,6α)-

Other names: Tricyclo[4.3.1.1

Inchi: InChI=1S/C11H16/c1-2-8-6-9(3-1)11-5-4-10(8)7-11/h4-5,8-11H,1-3,6-7H2

InchiKey: JPAKHMXDXKQUSA-UHFFFAOYSA-N

Formula: C11H16

SMILES: C1=CC2CC1C1CCCC2C1

Mol. weight [g/mol]: 148.25

Physical Properties

Property code	Value	Unit	Source
hf	33.54	kJ/mol	Cheméo Relay (1.0)
hfus	16.74	kJ/mol	Joback Method
hvap	50.58	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	NIST Webbook
ie	8.68	eV	NIST Webbook
logp	2.999		Crippen Method
mcvol	128.970	ml/mol	McGowan Method
tb	478.93	K	Cheméo Relay (1.0)
tf	371.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.53	J/mol×K	474.33	Joback Method
cpg	325.08	J/mol×K	511.21	Joback Method
cpg	345.10	J/mol×K	548.09	Joback Method
cpg	363.69	J/mol×K	584.97	Joback Method
cpg	380.95	J/mol×K	621.85	Joback Method
cpg	396.98	J/mol×K	658.72	Joback Method
cpg	411.89	J/mol×K	695.60	Joback Method
dvisc	0.0008654	Pa×s	257.03	Joback Method
dvisc	0.0009159	Pa×s	293.25	Joback Method
dvisc	0.0009573	Pa×s	329.46	Joback Method
dvisc	0.0009919	Pa×s	365.68	Joback Method
dvisc	0.0010212	Pa×s	401.90	Joback Method

dvisc	0.0010463	Pa×s	438.11	Joback Method
dvisc	0.0010680	Pa×s	474.33	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85523042&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

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point