Tricyclo[4.3.1.1(2,5)]undec-3-en-10-ol, stereoisomer

Inchi: InChI=1S/C11H16O/c12-11-9-2-1-3-10(11)8-5-4-7(9)6-8/h4-5,7-12H,1-3,6H2
InchiKey: XKEDIGAHBBTICC-UHFFFAOYSA-N
Formula: C11H16O
SMILES: OC1C2CCCC1C1C=CC2C1
Mol. weight [g/mol]: 164.24
CAS: 70220-95-0

Physical Properties

Property code	Value	Unit	Source
gf	77.51	kJ/mol	Joback Method
hf	-199.42	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
ie	8.40	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-2.37		Crippen Method
logp	1.969		Crippen Method
mcvol	134.840	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	561.84	K	Joback Method
tc	767.41	K	Joback Method
tf	313.61	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.26	J/mol×K	561.84	Joback Method
cpg	389.72	J/mol×K	596.10	Joback Method
cpg	406.04	J/mol×K	630.36	Joback Method
cpg	421.30	J/mol×K	664.62	Joback Method
cpg	435.57	J/mol×K	698.89	Joback Method
cpg	448.93	J/mol×K	733.15	Joback Method
cpg	461.45	J/mol×K	767.41	Joback Method

dvisc	0.0056192	Pa×s	313.61	Joback Method
dvisc	0.0033975	Pa×s	354.98	Joback Method
dvisc	0.0022818	Pa×s	396.35	Joback Method
dvisc	0.0016522	Pa×s	437.72	Joback Method
dvisc	0.0012649	Pa×s	479.10	Joback Method
dvisc	0.0010104	Pa×s	520.47	Joback Method
dvisc	0.0008343	Pa×s	561.84	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=C70220950&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
ie:	Ionization energy
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