Tricyclo[4.3.1.12,5]undec-3-en-10-ol, 10-methyl-, stereoisomer

Other names: 10-Methyltricyclo[4.3.1.1(2,5)]undec-3-en-10-ol
Inchi: InChI=1S/C12H18O/c1-12(13)10-3-2-4-11(12)9-6-5-8(10)7-9/h5-6,8-11,13H,2-4,7H2,1H3
InchiKey: GCFBIUOSKKLHSD-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC1(O)C2CCCC1C1C=CC2C1
Mol. weight [g/mol]: 178.27
CAS: 70220-96-1

Physical Properties

Property code	Value	Unit	Source
gf	80.44	kJ/mol	Joback Method
hf	-204.82	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	57.59	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.73	eV	NIST Webbook
log10ws	-2.79		Crippen Method
logp	2.360		Crippen Method
mcvol	148.930	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	584.96	K	Joback Method
tc	795.17	K	Joback Method
tf	348.78	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.78	J/mol×K	584.96	Joback Method
cpg	438.42	J/mol×K	620.00	Joback Method
cpg	454.91	J/mol×K	655.03	Joback Method
cpg	470.39	J/mol×K	690.07	Joback Method
cpg	485.04	J/mol×K	725.10	Joback Method
cpg	499.01	J/mol×K	760.14	Joback Method

cpg	512.46	J/mol×K	795.17	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=C70220961&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
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

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