9-Methyltricyclo[4.2.1.1(2,5)]deca-3,7-diene-9,10-d

Inchi: InChI=1S/C11H14O2/c1-11(13)8-4-5-9(11)7-3-2-6(8)10(7)12/h2-10,12-13H,1H3
InchiKey: OLANDCXXFRSOLN-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: CC1(O)C2C=CC1C1C=CC2C1O
Mol. weight [g/mol]: 178.23
CAS: 78323-73-6

Physical Properties

Property code	Value	Unit	Source
gf	-30.45	kJ/mol	Joback Method
hf	-292.81	kJ/mol	Joback Method
hfus	24.09	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	0.716		Crippen Method
mcvol	136.410	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	1299.00		NIST Webbook
rinpol	1299.00		NIST Webbook
tb	644.48	K	Joback Method
tc	839.79	K	Joback Method
tf	398.37	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.81	J/mol×K	644.48	Joback Method
cpg	421.26	J/mol×K	677.03	Joback Method
cpg	433.05	J/mol×K	709.58	Joback Method
cpg	444.31	J/mol×K	742.13	Joback Method
cpg	455.16	J/mol×K	774.68	Joback Method
cpg	465.74	J/mol×K	807.24	Joback Method
cpg	476.18	J/mol×K	839.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78323736&Units=SI
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

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
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

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