13-nor-Eremophila-1(10),6-dien-11-one

Inchi: InChI=1S/C14H20O/c1-10-5-4-6-13-8-7-12(11(2)15)9-14(10,13)3/h6,9-10H,4-5,7-8H2,1-3

InchiKey: KPRMOLFSYHPJAW-IINYFYTJSA-N

Formula: C14H20O

SMILES: CC(=O)C1=CC2(C)C(=CCCC2C)CC1

Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	46.35	kJ/mol	Joback Method
hf	-216.05	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.658		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
ripol	2209.00		NIST Webbook
tb	612.67	K	Joback Method
tc	843.52	K	Joback Method
tf	369.73	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.70	J/mol×K	612.67	Joback Method
cpg	494.14	J/mol×K	651.14	Joback Method
cpg	512.39	J/mol×K	689.62	Joback Method
cpg	529.59	J/mol×K	728.09	Joback Method
cpg	545.93	J/mol×K	766.57	Joback Method
cpg	561.56	J/mol×K	805.04	Joback Method
cpg	576.65	J/mol×K	843.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198673&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume