

13-nor-7,8-Epoxy-eremophil-1(10)-en-11-one

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H20O2/c1-9-5-4-6-11-7-12-14(16-12,10(2)15)8-13(9,11)3/h6,9,12H,4-5,7-8H

OQXGSYYUEPULKW-WTDIUWLJSA-N

C14H20O2

CC(=O)C12CC3(C)C(=CCCC3C)CC1O2

220.31

Physical Properties

Property code	Value	Unit	Source
gf	11.65	kJ/mol	Joback Method
hf	-314.34	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	56.44	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.869		Crippen Method
mcvol	178.680	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1653.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2350.00		NIST Webbook
tb	629.25	K	Joback Method
tc	863.72	K	Joback Method
tf	427.66	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.15	J/mol×K	629.25	Joback Method
cpg	529.11	J/mol×K	668.33	Joback Method
cpg	547.00	J/mol×K	707.41	Joback Method
cpg	564.13	J/mol×K	746.48	Joback Method
cpg	580.86	J/mol×K	785.56	Joback Method
cpg	597.49	J/mol×K	824.64	Joback Method
cpg	614.37	J/mol×K	863.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rlnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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