12-nor-Ziza-6(13)-en-2-«alpha»-yl methyl ether

Inchi: InChI=1S/C15H24O/c1-10-11(2)14-5-4-13(9-16-3)15(14)7-6-12(10)8-15/h10,12-14H,2,4-
InchiKey: RUVLTBWURBAPEN-CTUGBOSBSA-N
Formula: C15H24O
SMILES: C=C1C(C)C2CCC3(C2)C(COC)CCC13
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	160.64	kJ/mol	Joback Method
hf	-220.27	kJ/mol	Joback Method
hfus	20.68	kJ/mol	Joback Method
hvap	49.87	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.651		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1567.00		NIST Webbook
tb	583.84	K	Joback Method
tc	796.83	K	Joback Method
tf	356.92	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.29	J/mol×K	583.84	Joback Method
cpg	555.76	J/mol×K	619.34	Joback Method
cpg	576.88	J/mol×K	654.84	Joback Method
cpg	596.82	J/mol×K	690.33	Joback Method
cpg	615.72	J/mol×K	725.83	Joback Method
cpg	633.74	J/mol×K	761.33	Joback Method
cpg	651.01	J/mol×K	796.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R236027&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume