«DELTA»-9,10-Eremophilen-11-ol

Inchi: InChI=1S/C15H26O/c1-11(10-16)13-7-8-14-6-4-5-12(2)15(14,3)9-13/h12-14,16H,1,4-10H
InchiKey: YFKUAXRWMHKXSN-UHFFFAOYSA-N
Formula: C15H26O
SMILES: C=C(CO)C1CCC2CCCC(C)C2(C)C1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	70.08	kJ/mol	Joback Method
hf	-294.00	kJ/mol	Joback Method
hfus	19.82	kJ/mol	Joback Method
hvap	63.82	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.778		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
ripol	2193.00		NIST Webbook
tb	652.80	K	Joback Method
tc	858.50	K	Joback Method
tf	341.13	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.68	J/mol×K	652.80	Joback Method
cpg	617.20	J/mol×K	687.08	Joback Method
cpg	636.65	J/mol×K	721.37	Joback Method
cpg	655.14	J/mol×K	755.65	Joback Method
cpg	672.80	J/mol×K	789.93	Joback Method
cpg	689.76	J/mol×K	824.21	Joback Method
cpg	706.14	J/mol×K	858.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R285519&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