Germacra-1(10),4,11(13)-trien-12-ol

Inchi: InChI=1S/C15H24O/c1-12-5-4-6-13(2)8-10-15(9-7-12)14(3)11-16/h5,8,15-16H,3-4,6-7,9-
InchiKey: NDZJCEAHBZKIDU-PUCIIUOCSA-N
Formula: C15H24O
SMILES: C=C(CO)C1CC=C(C)CCC=C(C)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	34.60	kJ/mol	Joback Method
hf	-267.22	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	68.10	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.008		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1673.00		NIST Webbook
tb	676.25	K	Joback Method
tc	885.84	K	Joback Method
tf	323.77	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.93	J/mol×K	676.25	Joback Method
cpg	592.16	J/mol×K	711.18	Joback Method
cpg	610.20	J/mol×K	746.11	Joback Method
cpg	627.06	J/mol×K	781.05	Joback Method
cpg	642.75	J/mol×K	815.98	Joback Method
cpg	657.28	J/mol×K	850.91	Joback Method
cpg	670.67	J/mol×K	885.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R572873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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