Bisabola-1(6),10-dien-trans-2,3-diol A

Inchi: InChI=1S/C15H26O2/c1-10(2)6-5-7-11(3)13-9-8-12(4)14(16)15(13)17/h6,8,11,13-17H,5,
InchiKey: SDAWXTDBEYZMMX-UZVIJOLCSA-N
Formula: C15H26O2
SMILES: CC(C)=CCCC(C)C1CC=C(C)C(O)C1O
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-99.63	kJ/mol	Joback Method
hf	-495.29	kJ/mol	Joback Method
hfus	32.96	kJ/mol	Joback Method
hvap	82.76	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.057		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
ripol	2623.00		NIST Webbook
tb	744.91	K	Joback Method
tc	931.25	K	Joback Method
tf	358.59	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.73	J/mol×K	744.91	Joback Method
cpg	675.30	J/mol×K	775.97	Joback Method
cpg	690.03	J/mol×K	807.02	Joback Method
cpg	703.93	J/mol×K	838.08	Joback Method
cpg	717.03	J/mol×K	869.13	Joback Method
cpg	729.38	J/mol×K	900.19	Joback Method
cpg	741.00	J/mol×K	931.25	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=R229648&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume