

Guaia-6-en-10-«beta»-ol

Inchi: InChI=1S/C15H26O/c1-9(2)12-7-5-10(3)13-8-6-11(4)14(13)15(12)16/h5,9,11-16H,6-8H2,
InchiKey: IBXHXDRJWNEGRB-MWHZVNNOSA-N
Formula: C15H26O
SMILES: CC1=CCC(C(C)C)C(O)C2C(C)CCC12
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	6.46	kJ/mol	Joback Method
hf	-404.19	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	65.82	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.632		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1621.00		NIST Webbook
tb	655.03	K	Joback Method
tc	853.48	K	Joback Method
tf	326.99	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.82	J/mol×K	655.03	Joback Method
cpg	623.31	J/mol×K	688.11	Joback Method
cpg	642.65	J/mol×K	721.18	Joback Method
cpg	660.88	J/mol×K	754.26	Joback Method
cpg	678.03	J/mol×K	787.33	Joback Method
cpg	694.13	J/mol×K	820.41	Joback Method
cpg	709.21	J/mol×K	853.48	Joback Method
dvisc	0.0061187	Pa×s	326.99	Joback Method
dvisc	0.0021270	Pa×s	381.66	Joback Method

dvisc	0.0009635	Pa×s	436.34	Joback Method
dvisc	0.0005207	Pa×s	491.01	Joback Method
dvisc	0.0003183	Pa×s	545.68	Joback Method
dvisc	0.0002128	Pa×s	600.36	Joback Method
dvisc	0.0001522	Pa×s	655.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R204025&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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