10-epi-«beta»-Eudesmol

Inchi: InChI=1S/C15H26O/c1-11-6-5-8-15(4)9-7-12(10-13(11)15)14(2,3)16/h12-13,16H,1,5-10H
InchiKey: BOPIMTNSYWYZOC-GZBFAFLISA-N
Formula: C15H26O
SMILES: C=C1CCCC2(C)CCC(C(C)(C)O)CC12
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	54.42	kJ/mol	Joback Method
hf	-313.81	kJ/mol	Joback Method
hfus	12.76	kJ/mol	Joback Method
hvap	63.58	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	656.84	K	Joback Method
tc	868.05	K	Joback Method
tf	377.19	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.18	J/mol×K	656.84	Joback Method
cpg	617.32	J/mol×K	692.04	Joback Method
cpg	636.34	J/mol×K	727.24	Joback Method
cpg	654.38	J/mol×K	762.45	Joback Method
cpg	671.60	J/mol×K	797.65	Joback Method
cpg	688.14	J/mol×K	832.85	Joback Method

cpg	704.15	J/mol×K	868.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R441511&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