7-epi-Amiteol

Inchi: InChI=1S/C15H28O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h11-13,16H,5-10H2
InchiKey: PWTWAHBPEXYEQQ-QPSCCSFWSA-N
Formula: C15H28O
SMILES: CC(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 224.38

Physical Properties

Property code	Value	Unit	Source
gf	-17.14	kJ/mol	Joback Method
hf	-399.68	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.000		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1646.00		NIST Webbook
ripol	2264.00		NIST Webbook
tb	656.04	K	Joback Method
tc	865.65	K	Joback Method
tf	365.75	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.08	J/mol×K	656.04	Joback Method
cpg	638.19	J/mol×K	690.98	Joback Method
cpg	658.35	J/mol×K	725.91	Joback Method
cpg	677.78	J/mol×K	760.85	Joback Method
cpg	696.66	J/mol×K	795.78	Joback Method
cpg	715.22	J/mol×K	830.72	Joback Method
cpg	733.64	J/mol×K	865.65	Joback Method

Sources

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=R585250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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