3 «alpha»-Hydroxy-6-asteriscene

Inchi: InChI=1S/C15H26O/c1-11-6-5-7-15(4,16)13-10-14(2,3)9-12(13)8-11/h6,12-13,16H,5,7-10
InchiKey: FNFDOMBAWBPKHS-XYBYXXFYSA-N
Formula: C15H26O
SMILES: CC1=CCCC(C)(O)C2CC(C)(C)CC2C1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	-6.47	kJ/mol	Joback Method
hf	-354.25	kJ/mol	Joback Method
hfus	14.84	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	664.89	K	Joback Method
tc	879.55	K	Joback Method
tf	390.51	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.53	J/mol×K	664.89	Joback Method
cpg	616.99	J/mol×K	700.67	Joback Method
cpg	636.59	J/mol×K	736.44	Joback Method
cpg	655.52	J/mol×K	772.22	Joback Method
cpg	673.99	J/mol×K	808.00	Joback Method
cpg	692.21	J/mol×K	843.77	Joback Method
cpg	710.38	J/mol×K	879.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421191&Units=SI

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