

Atracylenolid

Inchi: InChI=1S/C15H24O/c1-10(2)13-6-5-12(4)15(16)8-7-11(3)9-14(13)15/h5,9-10,13-14,16H,
InchiKey: YNLHYEKVZRPZOE-SNTRVMSOSA-N
Formula: C15H24O
SMILES: CC1=CC2C(C(C)C)CC=C(C)C2(O)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	36.72	kJ/mol	Joback Method
hf	-301.96	kJ/mol	Joback Method
hfus	19.48	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1723.00		NIST Webbook
tb	668.75	K	Joback Method
tc	876.49	K	Joback Method
tf	372.65	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.81	J/mol×K	668.75	Joback Method
cpg	591.21	J/mol×K	703.37	Joback Method
cpg	608.71	J/mol×K	738.00	Joback Method
cpg	625.43	J/mol×K	772.62	Joback Method
cpg	641.48	J/mol×K	807.25	Joback Method
cpg	657.00	J/mol×K	841.87	Joback Method
cpg	672.09	J/mol×K	876.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R432458&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
hvac:	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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