Dehydrosabinaketone

Inchi: InChI=1S/C9H12O/c1-6(2)9-4-3-8(10)7(9)5-9/h3-4,6-7H,5H2,1-2H3
InchiKey: IBMZINAPWMATGM-UHFFFAOYSA-N
Formula: C9H12O
SMILES: CC(C)C12C=CC(=O)C1C2
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
gf	45.84	kJ/mol	Joback Method
hf	-153.45	kJ/mol	Joback Method
hfus	6.25	kJ/mol	Joback Method
hvap	38.45	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.788		Crippen Method
mcvol	113.220	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1117.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1117.00		NIST Webbook
tb	485.58	K	Joback Method
tc	711.64	K	Joback Method
tf	304.95	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.88	J/mol×K	485.58	Joback Method
cpg	277.23	J/mol×K	523.26	Joback Method
cpg	291.37	J/mol×K	560.93	Joback Method
cpg	304.45	J/mol×K	598.61	Joback Method
cpg	316.63	J/mol×K	636.29	Joback Method

cpg	328.06	J/mol×K	673.97	Joback Method
cpg	338.90	J/mol×K	711.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R616963&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
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