5-Methyl-5-vinyltetrahydrofur-2-yl methyl ketone (arbusculone)

Inchi: InChI=1S/C9H14O2/c1-4-9(3)6-5-8(11-9)7(2)10/h4,8H,1,5-6H2,2-3H3
InchiKey: FBFSXARBCWGXJL-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: C=CC1(C)CCC(C(C)=O)O1
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-78.95	kJ/mol	Joback Method
hf	-292.86	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.699		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
ripol	1452.00		NIST Webbook
ripol	1492.00		NIST Webbook
tb	493.67	K	Joback Method
tc	708.12	K	Joback Method
tf	296.49	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.91	J/mol×K	493.67	Joback Method
cpg	312.55	J/mol×K	529.41	Joback Method
cpg	327.13	J/mol×K	565.15	Joback Method
cpg	340.75	J/mol×K	600.89	Joback Method
cpg	353.53	J/mol×K	636.63	Joback Method
cpg	365.57	J/mol×K	672.38	Joback Method
cpg	376.99	J/mol×K	708.12	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=R336048&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume