cis-Arbusculone

Inchi: InChI=1S/C9H14O2/c1-4-9(3)6-5-8(11-9)7(2)10/h4,8H,1,5-6H2,2-3H3/t8-,9+/m0/s1
InchiKey: FBFSXARBCWGXJL-DTWKUNHWSA-N
Formula: C9H14O2
SMILES: C=CC1(C)CCC(C(C)=O)O1
Mol. weight [g/mol]: 154.21
CAS: 56469-37-5

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
rinpol	1026.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1052.50		NIST Webbook
rinpol	1058.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1071.50		NIST Webbook

rinpol	1071.00		NIST Webbook
rinpol	1071.00		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

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=C56469364&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume