trans-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-/m1/s1
InchiKey: FBFSXARBCWGXJL-DTWKUNHWSA-N
Formula: C9H14O2
SMILES: C=C[C@]1(C)CC[C@H](C(C)=O)O1
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
hfus	16.07	kJ/mol	Joback Method
logp	1.699		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
rinpol	1039.00		NIST Webbook
rinpol	1071.50		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1071.00		NIST Webbook

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56469364&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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