Dehydroisocarveol

Inchi: InChI=1S/C10H18O/c1-6-8-4-7(5-9(6)11)10(8,2)3/h6-9,11H,4-5H2,1-3H3
InchiKey: REPVLJRCJUVQFA-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1C(O)CC2CC1C2(C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-22.72	kJ/mol	Joback Method
hf	-308.30	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	52.45	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.049		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1214.00		NIST Webbook
tb	524.36	K	Joback Method
tc	717.42	K	Joback Method
tf	306.82	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.48	J/mol×K	524.36	Joback Method
cpg	372.00	J/mol×K	556.54	Joback Method
cpg	387.53	J/mol×K	588.71	Joback Method
cpg	402.17	J/mol×K	620.89	Joback Method
cpg	416.03	J/mol×K	653.07	Joback Method
cpg	429.20	J/mol×K	685.24	Joback Method
cpg	441.78	J/mol×K	717.42	Joback Method

Sources

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=R610910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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