

dihydroachillene

Inchi:	InChI=1S/C10H18/c1-6-10(9(4)5)7-8(2)3/h6,8H,1,7H2,2-5H3
InchiKey:	SHAPROXLZFAPJP-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	C=CC(CC(C)C)=C(C)C
Mol. weight [g/mol]:	138.25

Physical Properties

Property code	Value	Unit	Source
gf	181.84	kJ/mol	Joback Method
hf	-31.94	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	36.91	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
ripol	1547.00		NIST Webbook
tb	428.36	K	Joback Method
tc	612.80	K	Joback Method
tf	152.70	K	Joback Method
vc	0.552	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.95	J/mol×K	428.36	Joback Method
cpg	299.33	J/mol×K	459.10	Joback Method
cpg	313.96	J/mol×K	489.84	Joback Method
cpg	327.88	J/mol×K	520.58	Joback Method

cpg	341.12	J/mol×K	551.32	Joback Method
cpg	353.71	J/mol×K	582.06	Joback Method
cpg	365.68	J/mol×K	612.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R332600&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

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