

Pinocampheol

Inchi: InChI=1S/C10H18O/c1-6-8-4-7(5-9(6)11)10(8,2)3/h6-9,11H,4-5H2,1-3H3/t6-,7?,8?,9-/m0
InchiKey: REPVLJRCJUVQFA-KRTGUUSXSA-N
Formula: C10H18O
SMILES: CC1C(O)CC2CC1C2(C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
hf	-256.69	kJ/mol	Cheméo Relay (1.0)
hfus	16.83	kJ/mol	Joback Method
hvap	72.75	kJ/mol	Cheméo Relay (1.0)
logp	2.049		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
rinpol	1140.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1167.00		NIST Webbook
tb	482.61	K	Cheméo Relay (1.0)
tf	393.75	K	Cheméo Relay (1.0)

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:	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=R206303&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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