

trans-Verbenol

Inchi: InChI=1S/C10H16O/c1-6-4-9(11)8-5-7(6)10(8,2)3/h4,7-9,11H,5H2,1-3H3/t7-,8+,9+/m0/s1

InchiKey: WONIGEXYPVIKFS-DJLDLDEBSA-N

Formula: C10H16O

SMILES: CC1=CC(O)C2CC1C2(C)C

Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
hfus	16.59	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Cheméo Relay (1.0)
ie	8.72	eV	Cheméo Relay (1.0)
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
rinpol	1135.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1141.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1683.00		NIST Webbook
tb	486.43	K	Cheméo Relay (1.0)
tf	360.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.85	J/mol×K	533.17	Joback Method
cpg	351.53	J/mol×K	565.86	Joback Method
cpg	365.30	J/mol×K	598.55	Joback Method
cpg	378.26	J/mol×K	631.23	Joback Method
cpg	390.53	J/mol×K	663.92	Joback Method
cpg	402.21	J/mol×K	696.61	Joback Method
cpg	413.40	J/mol×K	729.30	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=U292863&Units=SI

Legend

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

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