

2-Caren-4-ol

Inchi:	InChI=1S/C10H16O/c1-6-4-7-9(8(11)5-6)10(7,2)3/h4,7-9,11H,5H2,1-3H3/t7-,8?,9-/m0/s1
InchiKey:	MLBMQUZCVXBGAS-SMOXQLQSSA-N
Formula:	C10H16O
SMILES:	CC1=CC2C(C(O)C1)C2(C)C
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
hfus	16.59	kJ/mol	Joback Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
ripol	1457.00		NIST Webbook
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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

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R516086&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
ripol:	Polar retention indices

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