

(E)-3(10)-CAREN-4-OL

Inchi:	InChI=1S/C10H16O/c1-6-4-7-8(5-9(6)11)10(7,2)3/h7-9,11H,1,4-5H2,2-3H3
InchiKey:	BKSIPWIAFSUQKX-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	C=C1CC2C(CC1O)C2(C)C
Mol. weight [g/mol]:	152.24

Physical Properties

Property code	Value	Unit	Source
hf	-169.82	kJ/mol	Cheméo Relay (1.0)
hfus	14.60	kJ/mol	Joback Method
hvap	75.12	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.96	J/mol×K	528.19	Joback Method
cpg	350.83	J/mol×K	560.67	Joback Method
cpg	364.79	J/mol×K	593.15	Joback Method
cpg	377.93	J/mol×K	625.63	Joback Method
cpg	390.35	J/mol×K	658.11	Joback Method
cpg	402.17	J/mol×K	690.59	Joback Method
cpg	413.48	J/mol×K	723.06	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=C1753351&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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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