

3-CAREN-10-AL

Inchi:	InChI=1S/C10H14O/c1-10(2)8-4-3-7(6-11)5-9(8)10/h3,6,8-9H,4-5H2,1-2H3
InchiKey:	UUEWWPMRAWHKBO-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC1(C)C2CC=C(C=O)CC21
Mol. weight [g/mol]:	150.22

Physical Properties

Property code	Value	Unit	Source
hf	-50.83	kJ/mol	Cheméo Relay (1.0)
hfus	13.72	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
ripol	1711.00		NIST Webbook
tb	487.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.50	J/mol×K	494.32	Joback Method
cpg	315.43	J/mol×K	530.04	Joback Method
cpg	330.16	J/mol×K	565.76	Joback Method
cpg	343.83	J/mol×K	601.47	Joback Method
cpg	356.59	J/mol×K	637.19	Joback Method
cpg	368.56	J/mol×K	672.91	Joback Method
cpg	379.90	J/mol×K	708.63	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151860&Units=SI
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):	

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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