

4,4-Dimethyl-2-methoxy-1-pentene

Other names:	4,4-Dimethyl-2-methoxy-1-pentene
Inchi:	InChI=1S/C8H16O/c1-7(9-5)6-8(2,3)4/h1,6H2,2-5H3
InchiKey:	LSHQWPNTYWCQMU-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C=C(CC(C)(C)C)OC
Mol. weight [g/mol]:	128.21

Physical Properties

Property code	Value	Unit	Source
hf	-254.50	kJ/mol	Cheméo Relay (1.0)
hfus	7.66	kJ/mol	Joback Method
hvap	37.96	kJ/mol	Cheméo Relay (1.0)
ie	8.38	eV	Cheméo Relay (1.0)
logp	2.583		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
tb	385.79	K	Cheméo Relay (1.0)
tf	182.96	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.78	J/mol×K	398.19	Joback Method
cpg	257.62	J/mol×K	428.47	Joback Method
cpg	270.82	J/mol×K	458.75	Joback Method
cpg	283.42	J/mol×K	489.02	Joback Method
cpg	295.43	J/mol×K	519.30	Joback Method
cpg	306.87	J/mol×K	549.58	Joback Method
cpg	317.76	J/mol×K	579.86	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C66017252&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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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