

2-Pentene, 2-methoxy-4,4-dimethyl-, (E)-

Inchi:	InChI=1S/C8H16O/c1-7(9-5)6-8(2,3)4/h6H,1-5H3/b7-6+
InchiKey:	WQPGFODYOJCBPR-VOTSOKGWSA-N
Formula:	C8H16O
SMILES:	COC(C)=CC(C)(C)C
Mol. weight [g/mol]:	128.21
CAS:	66017-29-6

Physical Properties

Property code	Value	Unit	Source
gf	-14.01	kJ/mol	Joback Method
hf	-241.99	kJ/mol	Joback Method
hfus	9.14	kJ/mol	Joback Method
hvap	34.55	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.583		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	405.67	K	Joback Method
tc	592.75	K	Joback Method
tf	185.53	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.28	J/mol×K	405.67	Joback Method
cpg	258.51	J/mol×K	436.85	Joback Method
cpg	272.02	J/mol×K	468.03	Joback Method
cpg	284.87	J/mol×K	499.21	Joback Method
cpg	297.06	J/mol×K	530.39	Joback Method
cpg	308.64	J/mol×K	561.57	Joback Method
cpg	319.62	J/mol×K	592.75	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66017296&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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