

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

Inchi:	InChI=1S/C6H12O/c1-4-5-6(2)7-3/h5H,4H2,1-3H3/b6-5-
InchiKey:	OMWMJRYDMINKPQ-WAYWQWQTSA-N
Formula:	C6H12O
SMILES:	CCC=C(C)OC
Mol. weight [g/mol]:	100.16
CAS:	41905-72-0

Physical Properties

Property code	Value	Unit	Source
gf	-33.69	kJ/mol	Joback Method
hf	-191.96	kJ/mol	Joback Method
hfus	11.38	kJ/mol	Joback Method
hvap	31.40	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.947		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	363.14	K	Joback Method
tc	540.00	K	Joback Method
tf	160.57	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.72	J/molxK	363.14	Joback Method
cpg	177.87	J/molxK	392.62	Joback Method
cpg	187.64	J/molxK	422.09	Joback Method
cpg	197.05	J/molxK	451.57	Joback Method
cpg	206.10	J/molxK	481.05	Joback Method
cpg	214.81	J/molxK	510.52	Joback Method
cpg	223.18	J/molxK	540.00	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C41905720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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