

Hept-2-ene, 2,4,4,6-tetramethyl-

Other names:	2-heptene, 2,4,4,6-tetramethyl-
Inchi:	InChI=1S/C11H22/c1-9(2)7-11(5,6)8-10(3)4/h7,10H,8H2,1-6H3
InchiKey:	JVBUFRVMYHEXRB-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	CC(C)=CC(C)(C)CC(C)C
Mol. weight [g/mol]:	154.29
CAS:	103982-58-7

Physical Properties

Property code	Value	Unit	Source
gf	113.81	kJ/mol	Joback Method
hf	-176.97	kJ/mol	Joback Method
hfus	12.20	kJ/mol	Joback Method
hvap	38.43	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	4.025		Crippen Method
mcvol	161.550	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	451.45	K	Joback Method
tc	638.50	K	Joback Method
tf	182.11	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.62	J/molxK	451.45	Joback Method
cpg	364.62	J/molxK	482.63	Joback Method
cpg	381.67	J/molxK	513.80	Joback Method
cpg	397.81	J/molxK	544.98	Joback Method
cpg	413.09	J/molxK	576.15	Joback Method
cpg	427.55	J/molxK	607.33	Joback Method
cpg	441.24	J/molxK	638.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C103982587&Units=SI

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
mcvol:	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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