2,4-Dimethyl 1,4-pentadiene

Inchi: InChI=1S/C7H12/c1-6(2)5-7(3)4/h1,3,5H2,2,4H3
InchiKey: ANKJYUSZUBOYDV-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=C(C)CC(=C)C
Mol. weight [g/mol]: 96.17
CAS: 4161-65-3

Physical Properties

Property code	Value	Unit	Source
gf	166.64	kJ/mol	Joback Method
hf	43.47	kJ/mol	Joback Method
hfus	8.71	kJ/mol	Joback Method
hvap	30.00	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.529		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	780.00		NIST Webbook
tb	352.68	K	Joback Method
tc	530.21	K	Joback Method
tf	137.21	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.04	J/mol×K	352.68	Joback Method
cpg	178.11	J/mol×K	382.27	Joback Method
cpg	188.68	J/mol×K	411.86	Joback Method
cpg	198.78	J/mol×K	441.44	Joback Method
cpg	208.43	J/mol×K	471.03	Joback Method
cpg	217.63	J/mol×K	500.62	Joback Method
cpg	226.41	J/mol×K	530.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4161653&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume