2,3-Dimethyl-1,4-pentadiene

Inchi: InChI=1S/C7H12/c1-5-7(4)6(2)3/h5,7H,1-2H2,3-4H3
InchiKey: SOKHGJZTJQMHEW-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=CC(C)C(=C)C
Mol. weight [g/mol]: 96.17
CAS: 758-86-1

Physical Properties

Property code	Value	Unit	Source
gf	172.75	kJ/mol	Joback Method
hf	47.98	kJ/mol	Joback Method
hfus	6.49	kJ/mol	Joback Method
hvap	29.53	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.385		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
ripol	1518.00		NIST Webbook
tb	352.36	K	Joback Method
tc	530.54	K	Joback Method
tf	136.17	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.83	J/mol×K	352.36	Joback Method
cpg	178.07	J/mol×K	382.06	Joback Method
cpg	188.81	J/mol×K	411.75	Joback Method
cpg	199.07	J/mol×K	441.45	Joback Method
cpg	208.86	J/mol×K	471.14	Joback Method
cpg	218.20	J/mol×K	500.84	Joback Method
cpg	227.10	J/mol×K	530.54	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=C758861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume