3-methylpenta-1,2-diene

Inchi: InChI=1S/C6H10/c1-4-6(3)5-2/h1,5H2,2-3H3
InchiKey: INFFCVIZNSUFGK-UHFFFAOYSA-N
Formula: C6H10
SMILES: C=C=C(C)CC
Mol. weight [g/mol]: 82.14
CAS: 7417-48-3

Physical Properties

Property code	Value	Unit	Source
gf	207.21	kJ/mol	Joback Method
hf	111.25	kJ/mol	Joback Method
hfus	10.84	kJ/mol	Joback Method
hvap	28.80	kJ/mol	Joback Method
ie	8.74 ± 0.05	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.128		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	336.51	K	Joback Method
tc	518.61	K	Joback Method
tf	148.17	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.82	J/mol×K	336.51	Joback Method
cpg	148.57	J/mol×K	366.86	Joback Method
cpg	157.04	J/mol×K	397.21	Joback Method
cpg	165.22	J/mol×K	427.56	Joback Method
cpg	173.13	J/mol×K	457.91	Joback Method
cpg	180.76	J/mol×K	488.26	Joback Method
cpg	188.13	J/mol×K	518.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7417483&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol376.mol

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
ie:	Ionization energy
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