2-Methyl-1, cis-3-pentadiene

Other names: (Z)-1,3-Pentadiene, 2-methyl-
1,3-Pentadiene, 2-methyl-, (Z)-
Inchi: InChI=1S/C6H10/c1-4-5-6(2)3/h4-5H,2H2,1,3H3/b5-4-
InchiKey: RCJMVGJKROQDCB-PLNGDYQASA-N
Formula: C6H10
SMILES: C=C(C)C=CC
Mol. weight [g/mol]: 82.14
CAS: 1501-60-6

Physical Properties

Property code	Value	Unit	Source
gf	159.15	kJ/mol	Joback Method
hf	65.69	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	28.32	kJ/mol	Joback Method
ie	8.65 ± 0.03	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	602.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	603.30		NIST Webbook
rinpol	602.90		NIST Webbook
rinpol	626.00		NIST Webbook
rinpol	628.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	629.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	629.00		NIST Webbook
tb	337.40	K	Joback Method
tc	517.19	K	Joback Method
tf	136.58	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.16	J/mol×K	337.40	Joback Method
cpg	142.08	J/mol×K	367.36	Joback Method
cpg	151.51	J/mol×K	397.33	Joback Method
cpg	160.47	J/mol×K	427.29	Joback Method
cpg	168.98	J/mol×K	457.26	Joback Method
cpg	177.07	J/mol×K	487.22	Joback Method
cpg	184.75	J/mol×K	517.19	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1501606&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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume