2,6-Dimethyl 1,7-octadiene

Inchi: InChI=1S/C10H18/c1-5-10(4)8-6-7-9(2)3/h5,10H,1-2,6-8H2,3-4H3
InchiKey: YXRZFCBXBJIBAP-UHFFFAOYSA-N
Formula: C10H18
SMILES: C=CC(C)CCCC(=C)C
Mol. weight [g/mol]: 138.25
CAS: 6874-35-7

Physical Properties

Property code	Value	Unit	Source
gf	198.01	kJ/mol	Joback Method
hf	-13.94	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	36.21	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.555		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	922.00		NIST Webbook
rinpol	933.00		NIST Webbook
tb	421.00	K	Joback Method
tc	596.95	K	Joback Method
tf	169.98	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.06	J/mol×K	421.00	Joback Method
cpg	297.83	J/mol×K	450.33	Joback Method
cpg	311.95	J/mol×K	479.65	Joback Method
cpg	325.44	J/mol×K	508.98	Joback Method
cpg	338.33	J/mol×K	538.30	Joback Method
cpg	350.64	J/mol×K	567.63	Joback Method
cpg	362.38	J/mol×K	596.95	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=C6874357&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
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