2,6-Dimethyl-1,3(E),5(Z),7-octatetraene

Inchi: InChI=1S/C10H14/c1-5-10(4)8-6-7-9(2)3/h5-8H,1-2H2,3-4H3/b7-6+,10-8+
InchiKey: HPZWSJQQCJZBBG-LQPGMRSMSA-N
Formula: C10H14
SMILES: C=CC(C)=CC=CC(=C)C
Mol. weight [g/mol]: 134.22

Physical Properties

Property code	Value	Unit	Source
gf	352.34	kJ/mol	Joback Method
hf	215.99	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	36.59	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.251		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
ripol	1446.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1446.00		NIST Webbook
tb	429.64	K	Joback Method
tc	623.05	K	Joback Method
tf	160.86	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.64	J/mol×K	429.64	Joback Method
cpg	266.80	J/mol×K	461.88	Joback Method
cpg	280.12	J/mol×K	494.11	Joback Method
cpg	292.65	J/mol×K	526.35	Joback Method
cpg	304.43	J/mol×K	558.58	Joback Method
cpg	315.52	J/mol×K	590.82	Joback Method
cpg	325.96	J/mol×K	623.05	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=R234254&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