(1-Methylenebut-2-enyl)benzene

Other names: 2-phenyl-1,3-pentadiene
Inchi: InChI=1S/C11H12/c1-3-7-10(2)11-8-5-4-6-9-11/h3-9H,2H2,1H3/b7-3+
InchiKey: MIUBQKCXRYVWFR-XVNBXDOJSA-N
Formula: C11H12
SMILES: C=C(C=CC)c1ccccc1
Mol. weight [g/mol]: 144.21
CAS: 70588-46-4

Physical Properties

Property code	Value	Unit	Source
gf	313.66	kJ/mol	Joback Method
hf	199.02	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.276		Crippen Method
mcvol	133.490	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1134.90		NIST Webbook
rinpol	1134.90		NIST Webbook
tb	478.48	K	Joback Method
tc	699.44	K	Joback Method
tf	219.35	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.71	J/mol×K	478.48	Joback Method
cpg	281.05	J/mol×K	515.31	Joback Method
cpg	295.33	J/mol×K	552.13	Joback Method
cpg	308.63	J/mol×K	588.96	Joback Method
cpg	321.00	J/mol×K	625.79	Joback Method
cpg	332.52	J/mol×K	662.61	Joback Method

cpg	343.23	J/mol×K	699.44	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=C70588464&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume