Benzene, 2,4-pentadiynyl-

Other names: Penta-2,4-diyn-1-ylbenzene
Inchi: InChI=1S/C11H8/c1-2-3-5-8-11-9-6-4-7-10-11/h1,4,6-7,9-10H,8H2
InchiKey: ZZGANZXITREHOP-UHFFFAOYSA-N
Formula: C11H8
SMILES: C#CC#CCc1ccccc1
Mol. weight [g/mol]: 140.18
CAS: 41268-41-1

Physical Properties

Property code	Value	Unit	Source
gf	580.02	kJ/mol	Joback Method
hf	530.36	kJ/mol	Joback Method
hfus	24.38	kJ/mol	Joback Method
hvap	44.37	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	1.866		Crippen Method
mcvol	124.890	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1285.70		NIST Webbook
tb	476.88	K	Joback Method
tc	725.71	K	Joback Method
tf	393.22	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.20	J/mol×K	476.88	Joback Method
cpg	249.68	J/mol×K	518.35	Joback Method
cpg	262.17	J/mol×K	559.82	Joback Method
cpg	273.73	J/mol×K	601.29	Joback Method
cpg	284.42	J/mol×K	642.76	Joback Method
cpg	294.31	J/mol×K	684.23	Joback Method
cpg	303.44	J/mol×K	725.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41268411&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

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