Capillene

Other names: Hexa-2,4-diyn-1-ylbenzene
Inchi: InChI=1S/C12H10/c1-2-3-4-6-9-12-10-7-5-8-11-12/h5,7-8,10-11H,9H2,1H3
InchiKey: WXQYRBLGGSLJHA-UHFFFAOYSA-N
Formula: C12H10
SMILES: CC#CC#CCc1ccccc1
Mol. weight [g/mol]: 154.21
CAS: 520-74-1

Physical Properties

Property code	Value	Unit	Source
gf	568.17	kJ/mol	Joback Method
hf	490.12	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	48.89	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.256		Crippen Method
mcvol	138.980	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	1501.20		NIST Webbook
tb	518.64	K	Joback Method
tc	776.81	K	Joback Method
tf	463.62	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.15	J/mol×K	518.64	Joback Method
cpg	293.30	J/mol×K	561.67	Joback Method
cpg	307.39	J/mol×K	604.70	Joback Method
cpg	320.50	J/mol×K	647.72	Joback Method
cpg	332.68	J/mol×K	690.75	Joback Method
cpg	343.98	J/mol×K	733.78	Joback Method
cpg	354.45	J/mol×K	776.81	Joback Method

Sources

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=C520741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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