Benzene, 3-heptynyl-

Other names: 3-Heptynyl-benzene
Inchi: InChI=1S/C13H16/c1-2-3-4-5-7-10-13-11-8-6-9-12-13/h6,8-9,11-12H,2-3,7,10H2,1H3
InchiKey: YEZVJYUTWUGSLO-UHFFFAOYSA-N
Formula: C13H16
SMILES: CCCC#CCCc1ccccc1
Mol. weight [g/mol]: 172.27
CAS: 56293-04-0

Physical Properties

Property code	Value	Unit	Source
gf	373.79	kJ/mol	Joback Method
hf	197.18	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	48.96	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.423		Crippen Method
mcvol	161.670	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
rinpol	230.20		NIST Webbook
tb	532.52	K	Joback Method
tc	754.72	K	Joback Method
tf	368.79	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.46	J/mol×K	532.52	Joback Method
cpg	375.46	J/mol×K	569.55	Joback Method
cpg	391.45	J/mol×K	606.59	Joback Method
cpg	406.46	J/mol×K	643.62	Joback Method
cpg	420.55	J/mol×K	680.65	Joback Method
cpg	433.76	J/mol×K	717.69	Joback Method
cpg	446.14	J/mol×K	754.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56293040&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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