(2-Propynyloxy)benzene

Inchi: InChI=1S/C9H8O/c1-2-8-10-9-6-4-3-5-7-9/h1,3-7H,8H2
InchiKey: AIQRJSXKXVZCJO-UHFFFAOYSA-N
Formula: C9H8O
SMILES: C#CCOc1ccccc1
Mol. weight [g/mol]: 132.16
CAS: 13045-88-0

Physical Properties

Property code	Value	Unit	Source
gf	255.38	kJ/mol	Joback Method
hf	167.12	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	40.17	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.699		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
ripol	1800.00		NIST Webbook
ripol	1800.00		NIST Webbook
tb	444.54	K	Joback Method
tc	666.28	K	Joback Method
tf	286.81	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.93	J/mol×K	444.54	Joback Method
cpg	220.90	J/mol×K	481.50	Joback Method
cpg	232.16	J/mol×K	518.45	Joback Method
cpg	242.73	J/mol×K	555.41	Joback Method
cpg	252.66	J/mol×K	592.37	Joback Method
cpg	261.95	J/mol×K	629.33	Joback Method
cpg	270.63	J/mol×K	666.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13045880&Units=SI

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