O-chlorophenyl propargyl ether

Inchi: InChI=1S/C9H7ClO/c1-2-7-11-9-6-4-3-5-8(9)10/h1,3-6H,7H2
InchiKey: CPJYMVHZHGCWOU-UHFFFAOYSA-N
Formula: C9H7ClO
SMILES: C#CCOc1ccccc1Cl
Mol. weight [g/mol]: 166.60
CAS: 17061-92-6

Physical Properties

Property code	Value	Unit	Source
gf	233.82	kJ/mol	Joback Method
hf	139.91	kJ/mol	Joback Method
hfus	21.08	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.352		Crippen Method
mcvol	123.420	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	486.95	K	Joback Method
tc	716.36	K	Joback Method
tf	329.25	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.35	J/mol×K	486.95	Joback Method
cpg	244.21	J/mol×K	525.18	Joback Method
cpg	254.40	J/mol×K	563.42	Joback Method
cpg	263.95	J/mol×K	601.65	Joback Method
cpg	272.89	J/mol×K	639.89	Joback Method
cpg	281.23	J/mol×K	678.12	Joback Method
cpg	289.00	J/mol×K	716.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17061926&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume