4-Tert-butylphenyl propargyl ether

Other names: Benzene, 1-(1,1-dimethylethyl)-4-(2-propynyloxy)-
Inchi: InChI=1S/C13H16O/c1-5-10-14-12-8-6-11(7-9-12)13(2,3)4/h1,6-9H,10H2,2-4H3
InchiKey: LCKMFILTJDWOQW-UHFFFAOYSA-N
Formula: C13H16O
SMILES: C#CCOc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 188.27
CAS: 48144-15-6

Physical Properties

Property code	Value	Unit	Source
gf	282.27	kJ/mol	Joback Method
hf	64.34	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	48.44	kJ/mol	Joback Method
ie	7.85 ± 0.02	eV	NIST Webbook
log10ws	-3.54		Crippen Method
logp	2.996		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	537.81	K	Joback Method
tc	760.93	K	Joback Method
tf	346.83	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.50	J/mol×K	537.81	Joback Method
cpg	402.32	J/mol×K	575.00	Joback Method
cpg	418.05	J/mol×K	612.18	Joback Method
cpg	432.74	J/mol×K	649.37	Joback Method
cpg	446.45	J/mol×K	686.56	Joback Method
cpg	459.24	J/mol×K	723.74	Joback Method
cpg	471.16	J/mol×K	760.93	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=C48144156&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
ie:	Ionization energy
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