Benzene, 2,4-dimethyl-1-(2-propynoxy)-

Inchi: InChI=1S/C11H12O/c1-4-7-12-11-6-5-9(2)8-10(11)3/h1,5-6,8H,7H2,2-3H3
InchiKey: CRJUIZSXKOAMAO-UHFFFAOYSA-N
Formula: C11H12O
SMILES: C#CCOc1ccc(C)cc1C
Mol. weight [g/mol]: 160.21
CAS: 116435-18-8

Physical Properties

Property code	Value	Unit	Source
gf	252.96	kJ/mol	Joback Method
hf	102.90	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.315		Crippen Method
mcvol	139.360	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
tb	500.26	K	Joback Method
tc	717.93	K	Joback Method
tf	334.39	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.09	J/mol×K	500.26	Joback Method
cpg	305.57	J/mol×K	536.54	Joback Method
cpg	318.37	J/mol×K	572.82	Joback Method
cpg	330.49	J/mol×K	609.09	Joback Method
cpg	341.96	J/mol×K	645.37	Joback Method
cpg	352.78	J/mol×K	681.65	Joback Method
cpg	362.99	J/mol×K	717.93	Joback Method

Sources

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=C116435188&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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