2H-Pyran, 2-(3-butynyloxy)tetrahydro-

Inchi: InChI=1S/C9H14O2/c1-2-3-7-10-9-6-4-5-8-11-9/h1,9H,3-8H2
InchiKey: ZQZSNKJFOFAJQX-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: C#CCCOC1CCCCO1
Mol. weight [g/mol]: 154.21
CAS: 40365-61-5

Physical Properties

Property code	Value	Unit	Source
gf	81.30	kJ/mol	Joback Method
hf	-147.09	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	42.84	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.553		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	464.36	K	Joback Method
tc	676.57	K	Joback Method
tf	294.34	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.80	J/mol×K	464.36	Joback Method
cpg	299.07	J/mol×K	499.73	Joback Method
cpg	314.53	J/mol×K	535.10	Joback Method
cpg	329.18	J/mol×K	570.47	Joback Method
cpg	343.04	J/mol×K	605.84	Joback Method
cpg	356.14	J/mol×K	641.20	Joback Method
cpg	368.47	J/mol×K	676.57	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.70	K	2.40	NIST Webbook

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=C40365615&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume