3-Phenyl-2-propyn-1-ol

Other names: 2-Propyn-1-ol, 3-phenyl-
3-phenyl-prop-2-yn-1-ol
Inchi: InChI=1S/C9H8O/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6,10H,8H2
InchiKey: NITUNGCLDSFVDL-UHFFFAOYSA-N
Formula: C9H8O
SMILES: OCC#Cc1ccccc1
Mol. weight [g/mol]: 132.16
CAS: 1504-58-1

Physical Properties

Property code	Value	Unit	Source
chl	-4764.70	kJ/mol	NIST Webbook
gf	203.29	kJ/mol	Joback Method
hf	127.51	kJ/mol	Joback Method
hfl	-49.80	kJ/mol	NIST Webbook
hfl	79.80 ± 4.00	kJ/mol	NIST Webbook
hfus	20.32	kJ/mol	Joback Method
hvap	56.73	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.030		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
tb	533.18	K	Joback Method
tc	753.32	K	Joback Method
tf	384.53	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.70	J/mol×K	533.18	Joback Method
cpg	241.14	J/mol×K	569.87	Joback Method
cpg	250.92	J/mol×K	606.56	Joback Method
cpg	260.06	J/mol×K	643.25	Joback Method

cpg	268.61	J/mol×K	679.94	Joback Method
cpg	276.58	J/mol×K	716.63	Joback Method
cpg	284.03	J/mol×K	753.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.50 ± 0.50	K	1.30	NIST Webbook

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=C1504581&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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