

1-Phenyloct-2-yn-1-ol

Inchi:	InChI=1S/C14H18O/c1-2-3-4-5-9-12-14(15)13-10-7-6-8-11-13/h6-8,10-11,14-15H,2-5H2
InchiKey:	GCCHIQSENJTUHA-UHFFFAOYSA-N
Formula:	C14H18O
SMILES:	CCCCC#CC(O)c1ccccc1
Mol. weight [g/mol]:	202.29
CAS:	62059-58-9

Physical Properties

Property code	Value	Unit	Source
chl	-7964.20	kJ/mol	NIST Webbook
gf	242.95	kJ/mol	Joback Method
hf	19.03	kJ/mol	Joback Method
hfl	177.00	kJ/mol	NIST Webbook
hfl	-117.40 ± 7.00	kJ/mol	NIST Webbook
hfus	29.74	kJ/mol	Joback Method
hvap	67.48	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.304		Crippen Method
mcvol	181.630	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	647.14	K	Joback Method
tc	854.02	K	Joback Method
tf	425.88	K	Joback Method
vc	0.686	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.73	J/molxK	647.14	Joback Method
cpg	481.39	J/molxK	681.62	Joback Method
cpg	495.18	J/molxK	716.10	Joback Method
cpg	508.14	J/molxK	750.58	Joback Method
cpg	520.32	J/molxK	785.06	Joback Method
cpg	531.76	J/molxK	819.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62059589&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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