

2-Phenylbicyclo[1,1,1]pentane-2-ol

Inchi: InChI=1S/C11H12O/c12-11(9-6-10(11)7-9)8-4-2-1-3-5-8/h1-5,9-10,12H,6-7H2
InchiKey: AITFJORBIAUXDI-UHFFFAOYSA-N
Formula: C11H12O
SMILES: OC1(c2ccccc2)C2CC1C2
Mol. weight [g/mol]: 160.21
CAS: 17684-73-0

Physical Properties

Property code	Value	Unit	Source
chs	-6092.30	kJ/mol	NIST Webbook
gf	137.73	kJ/mol	Joback Method
hf	135.80 ± 3.20	kJ/mol	NIST Webbook
hfs	48.70 ± 3.00	kJ/mol	NIST Webbook
hfus	15.52	kJ/mol	Joback Method
hsub	87.10 ± 1.10	kJ/mol	NIST Webbook
hsub	87.10	kJ/mol	NIST Webbook
hvap	57.23	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.914		Crippen Method
mcvol	126.240	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	574.72	K	Joback Method
tc	793.72	K	Joback Method
tf	348.75 ± 0.50	K	NIST Webbook
vc	0.481	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.79	J/mol×K	574.72	Joback Method
cpg	342.37	J/mol×K	611.22	Joback Method
cpg	354.89	J/mol×K	647.72	Joback Method
cpg	366.53	J/mol×K	684.22	Joback Method
cpg	377.47	J/mol×K	720.72	Joback Method

cpg	387.92	J/mol×K	757.22	Joback Method
cpg	398.05	J/mol×K	793.72	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=C17684730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

Latest version available from:

<https://www.chemeo.com/cid/61-168-8/2-Phenylbicyclo-1-1-1-pentane-2-ol.pdf>

Generated by Cheméo on 2024-04-28 23:02:04.36749228 +0000 UTC m=+16634573.288069596.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.