3-Benzylphenol

Inchi: InChI=1S/C13H12O/c14-13-8-4-7-12(10-13)9-11-5-2-1-3-6-11/h1-8,10,14H,9H2
InchiKey: JKFDELMIGLPLAX-UHFFFAOYSA-N
Formula: C13H12O
SMILES: Oc1cccc(Cc2ccccc2)c1
Mol. weight [g/mol]: 184.23
CAS: 22272-48-6

Physical Properties

Property code	Value	Unit	Source
chs	-6761.00	kJ/mol	NIST Webbook
gf	128.78	kJ/mol	Joback Method
hf	48.87	kJ/mol	NIST Webbook
hfs	-67.00	kJ/mol	NIST Webbook
hfus	23.29	kJ/mol	Joback Method
hsub	115.80	kJ/mol	NIST Webbook
hsub	115.90	kJ/mol	NIST Webbook
hvap	62.10	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.983		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	630.82	K	Joback Method
tc	885.31	K	Joback Method
tf	400.83	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.22	J/mol×K	630.82	Joback Method
cpg	391.93	J/mol×K	673.23	Joback Method
cpg	405.41	J/mol×K	715.65	Joback Method
cpg	417.82	J/mol×K	758.06	Joback Method
cpg	429.29	J/mol×K	800.48	Joback Method

cpg	440.00	J/mol×K	842.89	Joback Method
cpg	450.08	J/mol×K	885.31	Joback Method
dvisc	0.0010953	Pa×s	400.83	Joback Method
dvisc	0.0004472	Pa×s	439.16	Joback Method
dvisc	0.0002108	Pa×s	477.49	Joback Method
dvisc	0.0001111	Pa×s	515.82	Joback Method
dvisc	0.0000640	Pa×s	554.16	Joback Method
dvisc	0.0000396	Pa×s	592.49	Joback Method
dvisc	0.0000260	Pa×s	630.82	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22272486&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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