

3-Phenyl-1,3-pentandiol

Inchi:	InChI=1S/C11H16O2/c1-2-11(13,8-9-12)10-6-4-3-5-7-10/h3-7,12-13H,2,8-9H2,1H3
InchiKey:	GIYKXBLKTCZILH-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	CCC(O)(CCO)c1ccccc1
Mol. weight [g/mol]:	180.24
CAS:	93306-72-0

Physical Properties

Property code	Value	Unit	Source
gf	-116.65	kJ/mol	Joback Method
hf	-347.05	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.667		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
ripol	1824.00		NIST Webbook
ripol	1824.00		NIST Webbook
tb	658.89	K	Joback Method
tc	848.86	K	Joback Method
tf	364.21	K	Joback Method
vc	0.571	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.58	J/mol×K	658.89	Joback Method
cpg	426.85	J/mol×K	690.55	Joback Method
cpg	437.41	J/mol×K	722.21	Joback Method
cpg	447.32	J/mol×K	753.88	Joback Method
cpg	456.62	J/mol×K	785.54	Joback Method
cpg	465.36	J/mol×K	817.20	Joback Method
cpg	473.59	J/mol×K	848.86	Joback Method

dvisc	0.0079276	Paxs	364.21	Joback Method
dvisc	0.0015215	Paxs	413.32	Joback Method
dvisc	0.0004147	Paxs	462.44	Joback Method
dvisc	0.0001450	Paxs	511.55	Joback Method
dvisc	0.0000610	Paxs	560.66	Joback Method
dvisc	0.0000295	Paxs	609.78	Joback Method
dvisc	0.0000159	Paxs	658.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93306720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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