1,3-Propanediol, 2-(phenylmethyl)-

Inchi: InChI=1S/C10H14O2/c11-7-10(8-12)6-9-4-2-1-3-5-9/h1-5,10-12H,6-8H2
InchiKey: LODRGECCKZZTEQ-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: OCC(CO)Cc1ccccc1
Mol. weight [g/mol]: 166.22
CAS: 2612-30-8

Physical Properties

Property code	Value	Unit	Source
gf	-130.35	kJ/mol	Joback Method
hf	-322.94	kJ/mol	Joback Method
hfus	20.35	kJ/mol	Joback Method
hvap	73.10	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.830		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	638.80	K	Joback Method
tc	824.88	K	Joback Method
tf	341.00 ± 2.00	K	NIST Webbook
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.49	J/mol×K	638.80	Joback Method
cpg	374.01	J/mol×K	669.81	Joback Method
cpg	383.94	J/mol×K	700.83	Joback Method
cpg	393.30	J/mol×K	731.84	Joback Method
cpg	402.12	J/mol×K	762.86	Joback Method
cpg	410.42	J/mol×K	793.87	Joback Method
cpg	418.24	J/mol×K	824.88	Joback Method
dvisc	0.0180173	Pa×s	335.52	Joback Method
dvisc	0.0028092	Pa×s	386.07	Joback Method

dvisc	0.0006735	Pa×s	436.61	Joback Method
dvisc	0.0002172	Pa×s	487.16	Joback Method
dvisc	0.0000866	Pa×s	537.71	Joback Method
dvisc	0.0000405	Pa×s	588.25	Joback Method
dvisc	0.0000213	Pa×s	638.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2612308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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