2-Propanol, 2-phenyl, butanoate

Inchi: InChI=1S/C13H18O2/c1-4-8-12(14)15-13(2,3)11-9-6-5-7-10-11/h5-7,9-10H,4,8H2,1-3H3
InchiKey: PWJXAFDOZHNEHT-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCCC(=O)OC(C)(C)c1ccccc1
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-60.09	kJ/mol	Joback Method
hf	-328.67	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	54.67	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.265		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1476.00		NIST Webbook
ripol	1889.00		NIST Webbook
tb	596.58	K	Joback Method
tc	811.41	K	Joback Method
tf	337.27	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.48	J/mol×K	596.58	Joback Method
cpg	463.14	J/mol×K	632.38	Joback Method
cpg	478.72	J/mol×K	668.19	Joback Method
cpg	493.27	J/mol×K	703.99	Joback Method
cpg	506.83	J/mol×K	739.80	Joback Method
cpg	519.47	J/mol×K	775.60	Joback Method
cpg	531.22	J/mol×K	811.41	Joback Method
dvisc	0.0024771	Pa×s	337.27	Joback Method

dvisc	0.0011900	Pa×s	380.49	Joback Method
dvisc	0.0006639	Pa×s	423.71	Joback Method
dvisc	0.0004127	Pa×s	466.92	Joback Method
dvisc	0.0002780	Pa×s	510.14	Joback Method
dvisc	0.0001992	Pa×s	553.36	Joback Method
dvisc	0.0001498	Pa×s	596.58	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=R409295&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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/63-345-9/2-Propanol-2-phenyl-butanoate.pdf
Generated by Cheméo on 2024-10-12 02:45:08.212358958 +0000 UTC m=+3281970.849328208.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.