

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0011900	Paxs	380.49	Joback Method
dvisc	0.0006639	Paxs	423.71	Joback Method
dvisc	0.0004127	Paxs	466.92	Joback Method
dvisc	0.0002780	Paxs	510.14	Joback Method
dvisc	0.0001992	Paxs	553.36	Joback Method
dvisc	0.0001498	Paxs	596.58	Joback Method

Sources

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/ci9903071
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
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

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