

(Z)-4-Phenylbutan-2-yl acetate

Inchi:	InChI=1S/C12H14O2/c1-10(14-11(2)13)8-9-12-6-4-3-5-7-12/h3-10H,1-2H3/b9-8-
InchiKey:	DSWDNUYFUXOVBI-HJWRWDBZSA-N
Formula:	C12H14O2
SMILES:	CC(=O)OC(C)C=Cc1ccccc1
Mol. weight [g/mol]:	190.24

Physical Properties

Property code	Value	Unit	Source
gf	6.43	kJ/mol	Joback Method
hf	-187.34	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.651		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1374.00		NIST Webbook
tb	580.65	K	Joback Method
tc	800.23	K	Joback Method
tf	303.50	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.76	J/molxK	580.65	Joback Method
cpg	389.79	J/molxK	617.25	Joback Method
cpg	403.87	J/molxK	653.84	Joback Method
cpg	417.03	J/molxK	690.44	Joback Method
cpg	429.31	J/molxK	727.04	Joback Method
cpg	440.76	J/molxK	763.63	Joback Method
cpg	451.41	J/molxK	800.23	Joback Method
dvisc	0.0027204	Paxs	303.50	Joback Method
dvisc	0.0012128	Paxs	349.69	Joback Method

dvisc	0.0006529	Paxs	395.88	Joback Method
dvisc	0.0004000	Paxs	442.07	Joback Method
dvisc	0.0002689	Paxs	488.27	Joback Method
dvisc	0.0001936	Paxs	534.46	Joback Method
dvisc	0.0001469	Paxs	580.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341332&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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