

4-Oxo-4-phenylbutyric acid, butyl ester

Inchi:	InChI=1S/C14H18O3/c1-2-3-11-17-14(16)10-9-13(15)12-7-5-4-6-8-12/h4-8H,2-3,9-11H2
InchiKey:	AGWBSBAKSDAQBZ-UHFFFAOYSA-N
Formula:	C14H18O3
SMILES:	CCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]:	234.29

Physical Properties

Property code	Value	Unit	Source
gf	-183.43	kJ/mol	Joback Method
hf	-453.14	kJ/mol	Joback Method
hfus	30.44	kJ/mol	Joback Method
hvap	64.94	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.993		Crippen Method
mvol	193.370	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1881.00		NIST Webbook
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tb	676.56	K	Joback Method
tc	883.44	K	Joback Method
tf	396.05	K	Joback Method
vc	0.742	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.24	J/molxK	676.56	Joback Method
cpg	529.09	J/molxK	711.04	Joback Method
cpg	543.01	J/molxK	745.52	Joback Method
cpg	556.03	J/molxK	780.00	Joback Method
cpg	568.17	J/molxK	814.48	Joback Method
cpg	579.46	J/molxK	848.96	Joback Method
cpg	589.94	J/molxK	883.44	Joback Method
dvisc	0.0016695	Paxs	396.05	Joback Method

dvisc	0.0009099	Paxs	442.80	Joback Method
dvisc	0.0005569	Paxs	489.55	Joback Method
dvisc	0.0003713	Paxs	536.30	Joback Method
dvisc	0.0002642	Paxs	583.06	Joback Method
dvisc	0.0001977	Paxs	629.81	Joback Method
dvisc	0.0001540	Paxs	676.56	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=U405975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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