4-Oxo-4-phenylbutyric acid, pentyl ester

Inchi: InChI=1S/C15H20O3/c1-2-3-7-12-18-15(17)11-10-14(16)13-8-5-4-6-9-13/h4-6,8-9H,2-3,7
InchiKey: PIGYVSXCUZJDKU-UHFFFAOYSA-N
Formula: C15H20O3
SMILES: CCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
gf	-175.01	kJ/mol	Joback Method
hf	-473.78	kJ/mol	Joback Method
hfus	33.03	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.383		Crippen Method
mcvol	207.460	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	699.44	K	Joback Method
tc	903.67	K	Joback Method
tf	407.32	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.19	J/mol×K	699.44	Joback Method
cpg	582.45	J/mol×K	733.48	Joback Method
cpg	596.75	J/mol×K	767.52	Joback Method
cpg	610.13	J/mol×K	801.56	Joback Method
cpg	622.62	J/mol×K	835.59	Joback Method
cpg	634.23	J/mol×K	869.63	Joback Method
cpg	645.01	J/mol×K	903.67	Joback Method
dvisc	0.0015586	Pa×s	407.32	Joback Method

dvisc	0.0008373	Pa×s	456.01	Joback Method
dvisc	0.0005070	Pa×s	504.69	Joback Method
dvisc	0.0003354	Pa×s	553.38	Joback Method
dvisc	0.0002372	Pa×s	602.07	Joback Method
dvisc	0.0001767	Pa×s	650.75	Joback Method
dvisc	0.0001371	Pa×s	699.44	Joback Method

Sources

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=U405976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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