4-Oxo-4-phenylbutyric acid, heptyl ester

Inchi: InChI=1S/C17H24O3/c1-2-3-4-5-9-14-20-17(19)13-12-16(18)15-10-7-6-8-11-15/h6-8,10-
InchiKey: JZBJPXTZEBUACK-UHFFFAOYSA-N
Formula: C17H24O3
SMILES: CCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 276.37

Physical Properties

Property code	Value	Unit	Source
gf	-158.17	kJ/mol	Joback Method
hf	-515.06	kJ/mol	Joback Method
hfus	38.21	kJ/mol	Joback Method
hvap	71.61	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.163		Crippen Method
mcvol	235.640	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	745.20	K	Joback Method
tc	945.43	K	Joback Method
tf	429.86	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.68	J/mol×K	745.20	Joback Method
cpg	692.59	J/mol×K	778.57	Joback Method
cpg	707.50	J/mol×K	811.94	Joback Method
cpg	721.44	J/mol×K	845.32	Joback Method
cpg	734.46	J/mol×K	878.69	Joback Method
cpg	746.56	J/mol×K	912.06	Joback Method
cpg	757.80	J/mol×K	945.43	Joback Method
dvisc	0.0013307	Pa×s	429.86	Joback Method

dvisc	0.0006957	Pa×s	482.42	Joback Method
dvisc	0.0004131	Pa×s	534.97	Joback Method
dvisc	0.0002693	Pa×s	587.53	Joback Method
dvisc	0.0001883	Pa×s	640.09	Joback Method
dvisc	0.0001391	Pa×s	692.64	Joback Method
dvisc	0.0001072	Pa×s	745.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U405978&Units=SI

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