4-Oxo-4-phenylbutyric acid, hexyl ester

Inchi: InChI=1S/C16H22O3/c1-2-3-4-8-13-19-16(18)12-11-15(17)14-9-6-5-7-10-14/h5-7,9-10H,
InchiKey: IAEQYGYQJWEOJJ-UHFFFAOYSA-N
Formula: C16H22O3
SMILES: CCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 262.34

Physical Properties

Property code	Value	Unit	Source
gf	-166.59	kJ/mol	Joback Method
hf	-494.42	kJ/mol	Joback Method
hfus	35.62	kJ/mol	Joback Method
hvap	69.39	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.773		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
tb	722.32	K	Joback Method
tc	924.32	K	Joback Method
tf	418.59	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.37	J/mol×K	722.32	Joback Method
cpg	636.97	J/mol×K	755.99	Joback Method
cpg	651.60	J/mol×K	789.65	Joback Method
cpg	665.29	J/mol×K	823.32	Joback Method
cpg	678.06	J/mol×K	856.99	Joback Method
cpg	689.94	J/mol×K	890.65	Joback Method
cpg	700.97	J/mol×K	924.32	Joback Method
dvisc	0.0014448	Pa×s	418.59	Joback Method

dvisc	0.0007654	Pa×s	469.21	Joback Method
dvisc	0.0004589	Pa×s	519.83	Joback Method
dvisc	0.0003013	Pa×s	570.45	Joback Method
dvisc	0.0002119	Pa×s	621.08	Joback Method
dvisc	0.0001571	Pa×s	671.70	Joback Method
dvisc	0.0001215	Pa×s	722.32	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=U405977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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