4-Oxo-4-phenylbutyric acid, octyl ester

Inchi: InChI=1S/C18H26O3/c1-2-3-4-5-6-10-15-21-18(20)14-13-17(19)16-11-8-7-9-12-16/h7-9,
InchiKey: IZNTVVKVZSOEJM-UHFFFAOYSA-N
Formula: C18H26O3
SMILES: CCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 290.40

Physical Properties

Property code	Value	Unit	Source
gf	-149.75	kJ/mol	Joback Method
hf	-535.70	kJ/mol	Joback Method
hfus	40.80	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.553		Crippen Method
mcvol	249.730	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	768.08	K	Joback Method
tc	967.06	K	Joback Method
tf	441.13	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.06	J/mol×K	768.08	Joback Method
cpg	804.07	J/mol×K	933.89	Joback Method
cpg	791.77	J/mol×K	900.73	Joback Method
cpg	778.56	J/mol×K	867.57	Joback Method
cpg	764.39	J/mol×K	834.41	Joback Method
cpg	749.23	J/mol×K	801.24	Joback Method
cpg	815.48	J/mol×K	967.06	Joback Method
dvisc	0.0000942	Pa×s	768.08	Joback Method

dvisc	0.0001226	Pa×s	713.59	Joback Method
dvisc	0.0001667	Pa×s	659.10	Joback Method
dvisc	0.0002396	Pa×s	604.61	Joback Method
dvisc	0.0003701	Pa×s	550.11	Joback Method
dvisc	0.0006290	Pa×s	495.62	Joback Method
dvisc	0.0012185	Pa×s	441.13	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=U405979&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