4-Oxo-4-phenylbutyric acid, decyl ester

Inchi: InChI=1S/C20H30O3/c1-2-3-4-5-6-7-8-12-17-23-20(22)16-15-19(21)18-13-10-9-11-14-18
InchiKey: CTBKEQYDHQVHKU-UHFFFAOYSA-N
Formula: C20H30O3
SMILES: CCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 318.45

Physical Properties

Property code	Value	Unit	Source
gf	-132.91	kJ/mol	Joback Method
hf	-576.98	kJ/mol	Joback Method
hfus	45.98	kJ/mol	Joback Method
hvap	78.29	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.333		Crippen Method
mcvol	277.910	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	813.84	K	Joback Method
tc	1012.02	K	Joback Method
tf	463.67	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.69	J/mol×K	813.84	Joback Method
cpg	865.34	J/mol×K	846.87	Joback Method
cpg	880.92	J/mol×K	879.90	Joback Method
cpg	895.47	J/mol×K	912.93	Joback Method
cpg	909.03	J/mol×K	945.96	Joback Method
cpg	921.63	J/mol×K	978.99	Joback Method
cpg	933.31	J/mol×K	1012.02	Joback Method
dvisc	0.0010056	Pa×s	463.67	Joback Method

dvisc	0.0005068	Pa×s	522.03	Joback Method
dvisc	0.0002932	Pa×s	580.39	Joback Method
dvisc	0.0001875	Pa×s	638.75	Joback Method
dvisc	0.0001292	Pa×s	697.12	Joback Method
dvisc	0.0000943	Pa×s	755.48	Joback Method
dvisc	0.0000720	Pa×s	813.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405981&Units=SI
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

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