4-Oxo-4-phenylbutyric acid, dodecyl ester

Inchi: InChI=1S/C22H34O3/c1-2-3-4-5-6-7-8-9-10-14-19-25-22(24)18-17-21(23)20-15-12-11-13
InchiKey: WKJVPKOOWRIVEY-UHFFFAOYSA-N
Formula: C22H34O3
SMILES: CCCCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 346.50

Physical Properties

Property code	Value	Unit	Source
gf	-116.07	kJ/mol	Joback Method
hf	-618.26	kJ/mol	Joback Method
hfus	51.16	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.114		Crippen Method
mcvol	306.090	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	859.60	K	Joback Method
tc	1059.61	K	Joback Method
tf	486.21	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.70	J/mol×K	859.60	Joback Method
cpg	1042.39	J/mol×K	1026.28	Joback Method
cpg	1029.54	J/mol×K	992.94	Joback Method
cpg	1015.70	J/mol×K	959.61	Joback Method
cpg	1000.80	J/mol×K	926.27	Joback Method
cpg	984.82	J/mol×K	892.94	Joback Method
cpg	1054.27	J/mol×K	1059.61	Joback Method
dvisc	0.0000544	Pa×s	859.60	Joback Method

dvisc	0.0000716	Pa×s	797.37	Joback Method
dvisc	0.0000988	Pa×s	735.14	Joback Method
dvisc	0.0001446	Pa×s	672.90	Joback Method
dvisc	0.0002288	Pa×s	610.67	Joback Method
dvisc	0.0004018	Pa×s	548.44	Joback Method
dvisc	0.0008148	Pa×s	486.21	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=U405983&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