4-Oxo-4-phenylbutyric acid, hexadecyl ester

Inchi: InChI=1S/C26H42O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-23-29-26(28)22-21-25(27)24
InchiKey: KWBZBSHTLNLUQR-UHFFFAOYSA-N
Formula: C26H42O3
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 402.61

Physical Properties

Property code	Value	Unit	Source
gf	-82.39	kJ/mol	Joback Method
hf	-700.82	kJ/mol	Joback Method
hfus	61.52	kJ/mol	Joback Method
hvap	91.65	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	7.674		Crippen Method
mcvol	362.450	ml/mol	McGowan Method
pc	932.92	kPa	Joback Method
rinpol	3133.00		NIST Webbook
rinpol	3133.00		NIST Webbook
tb	951.12	K	Joback Method
tc	1164.44	K	Joback Method
tf	531.29	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.90	J/mol×K	951.12	Joback Method
cpg	1232.20	J/mol×K	986.67	Joback Method
cpg	1249.15	J/mol×K	1022.23	Joback Method
cpg	1264.83	J/mol×K	1057.78	Joback Method
cpg	1279.30	J/mol×K	1093.33	Joback Method
cpg	1292.63	J/mol×K	1128.89	Joback Method
cpg	1304.89	J/mol×K	1164.44	Joback Method
dvisc	0.0005114	Pa×s	531.29	Joback Method

dvisc	0.0002425	Pa×s	601.26	Joback Method
dvisc	0.0001344	Pa×s	671.23	Joback Method
dvisc	0.0000832	Pa×s	741.20	Joback Method
dvisc	0.0000560	Pa×s	811.18	Joback Method
dvisc	0.0000401	Pa×s	881.15	Joback Method
dvisc	0.0000302	Pa×s	951.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405987&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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