4-Oxo-4-phenylbutyric acid, pentadecyl ester

Inchi: InChI=1S/C25H40O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-22-28-25(27)21-20-24(26)23-18
InchiKey: RXWGJIYFTATTRN-UHFFFAOYSA-N
Formula: C25H40O3
SMILES: CCCCCCCCCCCCCCCOC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 388.58

Physical Properties

Property code	Value	Unit	Source
gf	-90.81	kJ/mol	Joback Method
hf	-680.18	kJ/mol	Joback Method
hfus	58.93	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.284		Crippen Method
mcvol	348.360	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
tb	928.24	K	Joback Method
tc	1136.87	K	Joback Method
tf	520.02	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.47	J/mol×K	928.24	Joback Method
cpg	1229.05	J/mol×K	1102.10	Joback Method
cpg	1215.85	J/mol×K	1067.33	Joback Method
cpg	1201.55	J/mol×K	1032.56	Joback Method
cpg	1186.10	J/mol×K	997.78	Joback Method
cpg	1169.42	J/mol×K	963.01	Joback Method
cpg	1241.21	J/mol×K	1136.87	Joback Method
dvisc	0.0000351	Pa×s	928.24	Joback Method

dvisc	0.0000465	Pa×s	860.20	Joback Method
dvisc	0.0000647	Pa×s	792.17	Joback Method
dvisc	0.0000959	Pa×s	724.13	Joback Method
dvisc	0.0001541	Pa×s	656.09	Joback Method
dvisc	0.0002764	Pa×s	588.06	Joback Method
dvisc	0.0005775	Pa×s	520.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405986&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