2-Phenylethyl docosanoate

Inchi: InChI=1S/C30H52O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-26-30(31)32
InchiKey: OCCJNJQOJXFKQO-UHFFFAOYSA-N
Formula: C30H52O2
SMILES: CCCCCCCCCCCCCCCCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 444.73
CAS: 104899-74-3

Physical Properties

Property code	Value	Unit	Source
gf	80.21	kJ/mol	Joback Method
hf	-670.80	kJ/mol	Joback Method
hfus	70.28	kJ/mol	Joback Method
hvap	93.81	kJ/mol	Joback Method
log10ws	-10.35		Crippen Method
logp	9.594		Crippen Method
mcvol	417.240	ml/mol	McGowan Method
pc	722.24	kPa	Joback Method
rinpol	3324.00		NIST Webbook
rinpol	3324.00		NIST Webbook
tb	988.77	K	Joback Method
tc	1215.45	K	Joback Method
tf	526.44	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1449.39	J/mol×K	988.77	Joback Method
cpg	1471.22	J/mol×K	1026.55	Joback Method
cpg	1491.45	J/mol×K	1064.33	Joback Method
cpg	1510.16	J/mol×K	1102.11	Joback Method
cpg	1527.47	J/mol×K	1139.89	Joback Method
cpg	1543.48	J/mol×K	1177.67	Joback Method
cpg	1558.27	J/mol×K	1215.45	Joback Method

dvisc	0.0004029	Pa×s	526.44	Joback Method
dvisc	0.0001708	Pa×s	603.49	Joback Method
dvisc	0.0000880	Pa×s	680.55	Joback Method
dvisc	0.0000519	Pa×s	757.60	Joback Method
dvisc	0.0000337	Pa×s	834.66	Joback Method
dvisc	0.0000236	Pa×s	911.71	Joback Method
dvisc	0.0000174	Pa×s	988.77	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104899743&Units=SI

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