Pimelic acid, dodecyl 3-phenylpropyl ester

Inchi: InChI=1S/C28H46O4/c1-2-3-4-5-6-7-8-9-10-17-24-31-27(29)22-15-12-16-23-28(30)32-25
InchiKey: NKUOCCVXRZAIEN-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-170.55	kJ/mol	Joback Method
hf	-874.32	kJ/mol	Joback Method
hfus	67.89	kJ/mol	Joback Method
hvap	98.51	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.577		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	824.31	kPa	Joback Method
rinpol	3142.00		NIST Webbook
rinpol	3142.00		NIST Webbook
tb	1019.30	K	Joback Method
tc	1252.65	K	Joback Method
tf	576.06	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.19	J/mol×K	1019.30	Joback Method
cpg	1388.60	J/mol×K	1058.19	Joback Method
cpg	1405.27	J/mol×K	1097.08	Joback Method
cpg	1420.28	J/mol×K	1135.98	Joback Method
cpg	1433.72	J/mol×K	1174.87	Joback Method
cpg	1445.65	J/mol×K	1213.76	Joback Method
cpg	1456.16	J/mol×K	1252.65	Joback Method
dvisc	0.0002698	Pa×s	576.06	Joback Method

dvisc	0.0001296	Pa×s	649.93	Joback Method
dvisc	0.0000723	Pa×s	723.81	Joback Method
dvisc	0.0000449	Pa×s	797.68	Joback Method
dvisc	0.0000303	Pa×s	871.55	Joback Method
dvisc	0.0000217	Pa×s	945.43	Joback Method
dvisc	0.0000163	Pa×s	1019.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416519&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

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