Pimelic acid, 4-methyl-2-pentyl phenethyl ester

Inchi: InChI=1S/C21H32O4/c1-17(2)16-18(3)25-21(23)13-9-5-8-12-20(22)24-15-14-19-10-6-4-7

InchiKey: LEOFOFKKQGTXHN-UHFFFAOYSA-N

Formula: C21H32O4

SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)OCCc1ccccc1

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-234.37	kJ/mol	Joback Method
hf	-740.40	kJ/mol	Joback Method
hfus	42.71	kJ/mol	Joback Method
hvap	82.15	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.701		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook
tb	858.26	K	Joback Method
tc	1061.58	K	Joback Method
tf	467.17	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.74	J/mol×K	858.26	Joback Method
cpg	955.38	J/mol×K	892.15	Joback Method
cpg	970.79	J/mol×K	926.03	Joback Method
cpg	985.01	J/mol×K	959.92	Joback Method
cpg	998.07	J/mol×K	993.81	Joback Method
cpg	1009.99	J/mol×K	1027.70	Joback Method
cpg	1020.81	J/mol×K	1061.58	Joback Method
dvisc	0.0008366	Pa×s	467.17	Joback Method

dvisc	0.0003680	Pa×s	532.35	Joback Method
dvisc	0.0001936	Pa×s	597.53	Joback Method
dvisc	0.0001156	Pa×s	662.71	Joback Method
dvisc	0.0000757	Pa×s	727.90	Joback Method
dvisc	0.0000531	Pa×s	793.08	Joback Method
dvisc	0.0000394	Pa×s	858.26	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=U416499&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

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