Pimelic acid, 3-phenylpropyl propyl ester

Inchi: InChI=1S/C19H28O4/c1-2-15-22-18(20)13-7-4-8-14-19(21)23-16-9-12-17-10-5-3-6-11-17
InchiKey: CAIBHFBKIJQJIE-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCCOC(=O)CCCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-246.33	kJ/mol	Joback Method
hf	-688.56	kJ/mol	Joback Method
hfus	44.58	kJ/mol	Joback Method
hvap	78.48	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.066		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2439.00		NIST Webbook
tb	813.38	K	Joback Method
tc	1012.05	K	Joback Method
tf	474.63	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.71	J/mol×K	813.38	Joback Method
cpg	835.71	J/mol×K	846.49	Joback Method
cpg	850.62	J/mol×K	879.60	Joback Method
cpg	864.47	J/mol×K	912.71	Joback Method
cpg	877.28	J/mol×K	945.83	Joback Method
cpg	889.08	J/mol×K	978.94	Joback Method
cpg	899.89	J/mol×K	1012.05	Joback Method
dvisc	0.0007727	Pa×s	474.63	Joback Method
dvisc	0.0004063	Pa×s	531.09	Joback Method

dvisc	0.0002418	Pa×s	587.55	Joback Method
dvisc	0.0001576	Pa×s	644.00	Joback Method
dvisc	0.0001100	Pa×s	700.46	Joback Method
dvisc	0.0000811	Pa×s	756.92	Joback Method
dvisc	0.0000623	Pa×s	813.38	Joback Method

Sources

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=U416508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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