

Pimelic acid, pentyl 3-phenylpropyl ester

Inchi:	InChI=1S/C21H32O4/c1-2-3-10-17-24-20(22)15-8-5-9-16-21(23)25-18-11-14-19-12-6-4-7
InchiKey:	QVLPSNQDIURNQC-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-229.49	kJ/mol	Joback Method
hf	-729.84	kJ/mol	Joback Method
hfus	49.76	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.846		Crippen Method
mvol	297.870	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinpol	2676.00		NIST Webbook
rinpol	2676.00		NIST Webbook
tb	859.14	K	Joback Method
tc	1059.46	K	Joback Method
tf	497.17	K	Joback Method
vc	1.151	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.74	J/molxK	859.14	Joback Method
cpg	954.16	J/molxK	892.53	Joback Method
cpg	969.42	J/molxK	925.91	Joback Method
cpg	983.54	J/molxK	959.30	Joback Method
cpg	996.55	J/molxK	992.69	Joback Method
cpg	1008.48	J/molxK	1026.07	Joback Method
cpg	1019.36	J/molxK	1059.46	Joback Method
dvisc	0.0006267	Paxs	497.17	Joback Method

dvisc	0.0003221	Paxs	557.50	Joback Method
dvisc	0.0001885	Paxs	617.83	Joback Method
dvisc	0.0001214	Paxs	678.15	Joback Method
dvisc	0.0000840	Paxs	738.48	Joback Method
dvisc	0.0000614	Paxs	798.81	Joback Method
dvisc	0.0000470	Paxs	859.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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