

Pimelic acid, butyl 3-phenylpropyl ester

Inchi:	InChI=1S/C20H30O4/c1-2-3-16-23-19(21)14-8-5-9-15-20(22)24-17-10-13-18-11-6-4-7-12
InchiKey:	RAWSNMXVOPHMOK-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCCCOC(=O)CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-237.91	kJ/mol	Joback Method
hf	-709.20	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.456		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinsol	2539.00		NIST Webbook
tb	836.26	K	Joback Method
tc	1035.40	K	Joback Method
tf	485.90	K	Joback Method
vc	1.095	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.33	J/molxK	836.26	Joback Method
cpg	894.55	J/molxK	869.45	Joback Method
cpg	909.64	J/molxK	902.64	Joback Method
cpg	923.63	J/molxK	935.83	Joback Method
cpg	936.55	J/molxK	969.02	Joback Method
cpg	948.42	J/molxK	1002.21	Joback Method
cpg	959.28	J/molxK	1035.40	Joback Method
dvisc	0.0006973	Paxs	485.90	Joback Method
dvisc	0.0003625	Paxs	544.29	Joback Method

dvisc	0.0002139	Paxs	602.69	Joback Method
dvisc	0.0001385	Paxs	661.08	Joback Method
dvisc	0.0000963	Paxs	719.47	Joback Method
dvisc	0.0000707	Paxs	777.87	Joback Method
dvisc	0.0000542	Paxs	836.26	Joback Method

Sources

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=U416510&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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