

Pimelic acid, isobutyl 3-phenylpropyl ester

Inchi:	InChI=1S/C20H30O4/c1-17(2)16-24-20(22)14-8-4-7-13-19(21)23-15-9-12-18-10-5-3-6-1
InchiKey:	ABXHZADKXGMHRD-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CC(C)COC(=O)CCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-240.35	kJ/mol	Joback Method
hf	-714.48	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	80.31	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.312		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	835.82	K	Joback Method
tc	1036.72	K	Joback Method
tf	470.90	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.85	J/molxK	835.82	Joback Method
cpg	895.20	J/molxK	869.30	Joback Method
cpg	910.39	J/molxK	902.79	Joback Method
cpg	924.45	J/molxK	936.27	Joback Method
cpg	937.41	J/molxK	969.75	Joback Method
cpg	949.30	J/molxK	1003.23	Joback Method
cpg	960.15	J/molxK	1036.72	Joback Method
dvisc	0.0008026	Paxs	470.90	Joback Method

dvisc	0.0003871	Paxs	531.72	Joback Method
dvisc	0.0002169	Paxs	592.54	Joback Method
dvisc	0.0001354	Paxs	653.36	Joback Method
dvisc	0.0000915	Paxs	714.18	Joback Method
dvisc	0.0000658	Paxs	775.00	Joback Method
dvisc	0.0000497	Paxs	835.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416509&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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