

Pimelic acid, isobutyl phenethyl ester

Inchi:	InChI=1S/C19H28O4/c1-16(2)15-23-19(21)12-8-4-7-11-18(20)22-14-13-17-9-5-3-6-10-17
InchiKey:	LCVGRBJWJYIPJW-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CC(C)COC(=O)CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-248.77	kJ/mol	Joback Method
hf	-693.84	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	78.09	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.922		Crippen Method
mvol	269.690	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	2366.00		NIST Webbook
tb	812.94	K	Joback Method
tc	1013.68	K	Joback Method
tf	459.63	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.24	J/molxK	812.94	Joback Method
cpg	836.40	J/molxK	846.40	Joback Method
cpg	851.44	J/molxK	879.85	Joback Method
cpg	865.38	J/molxK	913.31	Joback Method
cpg	878.26	J/molxK	946.77	Joback Method
cpg	890.09	J/molxK	980.22	Joback Method
cpg	900.91	J/molxK	1013.68	Joback Method
dvisc	0.0008938	Paxs	459.63	Joback Method
dvisc	0.0004358	Paxs	518.51	Joback Method

dvisc	0.0002460	Paxs	577.40	Joback Method
dvisc	0.0001544	Paxs	636.28	Joback Method
dvisc	0.0001048	Paxs	695.17	Joback Method
dvisc	0.0000756	Paxs	754.05	Joback Method
dvisc	0.0000572	Paxs	812.94	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=U416497&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

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