

Pimelic acid, ethyl phenethyl ester

Inchi:	InChI=1S/C17H24O4/c1-2-20-16(18)11-7-4-8-12-17(19)21-14-13-15-9-5-3-6-10-15/h3,5-
InchiKey:	MWPSQXOEDIWNCL-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CCOC(=O)CCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-263.17	kJ/mol	Joback Method
hf	-647.28	kJ/mol	Joback Method
hfus	39.40	kJ/mol	Joback Method
hvap	74.02	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.286		Crippen Method
mvol	241.510	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tb	767.62	K	Joback Method
tc	967.25	K	Joback Method
tf	452.09	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.09	J/molxK	767.62	Joback Method
cpg	720.60	J/molxK	800.89	Joback Method
cpg	735.10	J/molxK	834.16	Joback Method
cpg	748.60	J/molxK	867.43	Joback Method
cpg	761.13	J/molxK	900.71	Joback Method
cpg	772.69	J/molxK	933.98	Joback Method
cpg	783.32	J/molxK	967.25	Joback Method
dvisc	0.0009355	Paxs	452.09	Joback Method

dvisc	0.0005043	Paxs	504.68	Joback Method
dvisc	0.0003054	Paxs	557.27	Joback Method
dvisc	0.0002017	Paxs	609.86	Joback Method
dvisc	0.0001423	Paxs	662.44	Joback Method
dvisc	0.0001057	Paxs	715.03	Joback Method
dvisc	0.0000817	Paxs	767.62	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416495&Units=SI

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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