

Pimelic acid, ethyl 2-methylphenyl ester

Inchi:	InChI=1S/C16H22O4/c1-3-19-15(17)11-5-4-6-12-16(18)20-14-10-8-7-9-13(14)2/h7-10H,3
InchiKey:	PYDHBWCSMZACLH-UHFFFAOYSA-N
Formula:	C16H22O4
SMILES:	CCOC(=O)CCCCC(=O)Oc1ccccc1C
Mol. weight [g/mol]:	278.34

Physical Properties

Property code	Value	Unit	Source
gf	-281.22	kJ/mol	Joback Method
hf	-638.11	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.414		Crippen Method
mvol	227.420	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2152.00		NIST Webbook
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tb	749.72	K	Joback Method
tc	951.49	K	Joback Method
tf	453.34	K	Joback Method
vc	0.872	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.45	J/molxK	749.72	Joback Method
cpg	663.58	J/molxK	783.35	Joback Method
cpg	677.73	J/molxK	816.98	Joback Method
cpg	690.92	J/molxK	850.61	Joback Method
cpg	703.17	J/molxK	884.24	Joback Method
cpg	714.48	J/molxK	917.86	Joback Method
cpg	724.87	J/molxK	951.49	Joback Method
dvisc	0.0008522	Paxs	453.34	Joback Method

dvisc	0.0004919	Paxs	502.74	Joback Method
dvisc	0.0003132	Paxs	552.13	Joback Method
dvisc	0.0002148	Paxs	601.53	Joback Method
dvisc	0.0001560	Paxs	650.93	Joback Method
dvisc	0.0001185	Paxs	700.32	Joback Method
dvisc	0.0000934	Paxs	749.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416482&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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