Adipic acid, ethyl 2-propylphenyl ester

Inchi: InChI=1S/C17H24O4/c1-3-9-14-10-5-6-11-15(14)21-17(19)13-8-7-12-16(18)20-4-2/h5-6,
InchiKey: PVHUSFVCWXXJMT-UHFFFAOYSA-N
Formula: C17H24O4
SMILES: CCCc1ccccc1OC(=O)CCCCC(=O)OCC
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-272.80	kJ/mol	Joback Method
hf	-658.75	kJ/mol	Joback Method
hfus	39.01	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.668		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2086.00		NIST Webbook
tb	772.60	K	Joback Method
tc	973.04	K	Joback Method
tf	464.61	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.35	J/mol×K	772.60	Joback Method
cpg	771.51	J/mol×K	939.63	Joback Method
cpg	760.03	J/mol×K	906.23	Joback Method
cpg	747.59	J/mol×K	872.82	Joback Method
cpg	734.18	J/mol×K	839.41	Joback Method
cpg	719.77	J/mol×K	806.01	Joback Method
cpg	782.03	J/mol×K	973.04	Joback Method
dvisc	0.0000821	Pa×s	772.60	Joback Method
dvisc	0.0001047	Pa×s	721.27	Joback Method

dvisc	0.0001384	Pa×s	669.94	Joback Method
dvisc	0.0001917	Pa×s	618.61	Joback Method
dvisc	0.0002816	Pa×s	567.27	Joback Method
dvisc	0.0004467	Pa×s	515.94	Joback Method
dvisc	0.0007844	Pa×s	464.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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