Isophthalic acid, phenyl propyl ester

Inchi: InChI=1S/C17H16O4/c1-2-11-20-16(18)13-7-6-8-14(12-13)17(19)21-15-9-4-3-5-10-15/h3
InchiKey: YGKACTWREOOWKZ-UHFFFAOYSA-N
Formula: C17H16O4
SMILES: CCCOC(=O)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]: 284.31

Physical Properties

Property code	Value	Unit	Source
gf	-160.39	kJ/mol	Joback Method
hf	-422.22	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	76.96	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.473		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	799.28	K	Joback Method
tc	1031.24	K	Joback Method
tf	491.03	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.85	J/mol×K	799.28	Joback Method
cpg	626.62	J/mol×K	837.94	Joback Method
cpg	639.17	J/mol×K	876.60	Joback Method
cpg	650.51	J/mol×K	915.26	Joback Method
cpg	660.68	J/mol×K	953.92	Joback Method
cpg	669.72	J/mol×K	992.58	Joback Method
cpg	677.64	J/mol×K	1031.24	Joback Method
dvisc	0.0006762	Pa×s	491.03	Joback Method

dvisc	0.0004045	Pa×s	542.40	Joback Method
dvisc	0.0002645	Pa×s	593.78	Joback Method
dvisc	0.0001851	Pa×s	645.15	Joback Method
dvisc	0.0001365	Pa×s	696.53	Joback Method
dvisc	0.0001050	Pa×s	747.90	Joback Method
dvisc	0.0000835	Pa×s	799.28	Joback Method

Sources

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=U344355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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