3-Phenylpropanoic anhydride

Inchi: InChI=1S/C18H18O3/c19-17(13-11-15-7-3-1-4-8-15)21-18(20)14-12-16-9-5-2-6-10-16/h1
InchiKey: SQAHPYZABTWPNY-UHFFFAOYSA-N
Formula: C18H18O3
SMILES: O=C(CCc1ccccc1)OC(=O)CCc1ccccc1
Mol. weight [g/mol]: 282.33

Physical Properties

Property code	Value	Unit	Source
gf	-37.34	kJ/mol	Joback Method
hf	-299.17	kJ/mol	Joback Method
hfus	34.84	kJ/mol	Joback Method
hvap	76.12	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.322		Crippen Method
mcvol	225.970	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	2295.70		NIST Webbook
rinpol	2295.70		NIST Webbook
tb	794.76	K	Joback Method
tc	1024.98	K	Joback Method
tf	467.55	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.62	J/mol×K	794.76	Joback Method
cpg	704.16	J/mol×K	986.61	Joback Method
cpg	694.06	J/mol×K	948.24	Joback Method
cpg	682.92	J/mol×K	909.87	Joback Method
cpg	670.67	J/mol×K	871.50	Joback Method
cpg	657.26	J/mol×K	833.13	Joback Method
cpg	713.28	J/mol×K	1024.98	Joback Method
dvisc	0.0000955	Pa×s	794.76	Joback Method

dvisc	0.0001225	Pa×s	740.22	Joback Method
dvisc	0.0001635	Pa×s	685.69	Joback Method
dvisc	0.0002294	Pa×s	631.15	Joback Method
dvisc	0.0003431	Pa×s	576.62	Joback Method
dvisc	0.0005581	Pa×s	522.09	Joback Method
dvisc	0.0010172	Pa×s	467.55	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333896&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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