Propyl 3,4,5-triacetoxybenzoate

Inchi: InChI=1S/C16H18O8/c1-5-6-21-16(20)12-7-13(22-9(2)17)15(24-11(4)19)14(8-12)23-10(3
InchiKey: SZGQQTUWXGYOOA-UHFFFAOYSA-N
Formula: C16H18O8
SMILES: CCCOC(=O)c1cc(OC(C)=O)c(OC(C)=O)c(OC(C)=O)c1
Mol. weight [g/mol]: 338.31

Physical Properties

Property code	Value	Unit	Source
gf	-768.32	kJ/mol	Joback Method
hf	-1150.65	kJ/mol	Joback Method
hfus	41.22	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.029		Crippen Method
mcvol	242.300	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2225.00		NIST Webbook
tb	912.26	K	Joback Method
tc	1129.47	K	Joback Method
tf	622.70	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.77	J/mol×K	912.26	Joback Method
cpg	735.00	J/mol×K	948.46	Joback Method
cpg	743.87	J/mol×K	984.66	Joback Method
cpg	751.36	J/mol×K	1020.87	Joback Method
cpg	757.43	J/mol×K	1057.07	Joback Method
cpg	762.04	J/mol×K	1093.27	Joback Method
cpg	765.16	J/mol×K	1129.47	Joback Method
dvisc	0.0002582	Pa×s	622.70	Joback Method

dvisc	0.0001791	Pa×s	670.96	Joback Method
dvisc	0.0001304	Pa×s	719.22	Joback Method
dvisc	0.0000988	Pa×s	767.48	Joback Method
dvisc	0.0000774	Pa×s	815.74	Joback Method
dvisc	0.0000623	Pa×s	864.00	Joback Method
dvisc	0.0000513	Pa×s	912.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373065&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
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