Propyl glucuronide, methyl ester, triacetate

Inchi: InChI=1S/C16H24O10/c1-6-7-22-16-14(25-10(4)19)12(24-9(3)18)11(23-8(2)17)13(26-16
InchiKey: VDBRYEIACQHBSB-UHFFFAOYSA-N
Formula: C16H24O10
SMILES: CCCOC1OC(C(=O)OC)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 376.36

Physical Properties

Property code	Value	Unit	Source
gf	-1049.35	kJ/mol	Joback Method
hf	-1644.03	kJ/mol	Joback Method
hfus	53.63	kJ/mol	Joback Method
hvap	93.95	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.106		Crippen Method
mcvol	266.940	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	920.88	K	Joback Method
tc	1133.72	K	Joback Method
tf	597.94	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.52	J/mol×K	920.88	Joback Method
cpg	911.94	J/mol×K	956.35	Joback Method
cpg	922.45	J/mol×K	991.83	Joback Method
cpg	930.98	J/mol×K	1027.30	Joback Method
cpg	937.47	J/mol×K	1062.77	Joback Method
cpg	941.86	J/mol×K	1098.25	Joback Method
cpg	944.08	J/mol×K	1133.72	Joback Method
dvisc	0.0004734	Pa×s	597.94	Joback Method

dvisc	0.0003228	Pa×s	651.76	Joback Method
dvisc	0.0002333	Pa×s	705.59	Joback Method
dvisc	0.0001766	Pa×s	759.41	Joback Method
dvisc	0.0001387	Pa×s	813.23	Joback Method
dvisc	0.0001123	Pa×s	867.06	Joback Method
dvisc	0.0000931	Pa×s	920.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554657&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