Butyl glucuronide, methyl ester, triacetate

Inchi: InChI=1S/C17H26O10/c1-6-7-8-23-17-15(26-11(4)20)13(25-10(3)19)12(24-9(2)18)14(27
InchiKey: PFVMVZJERPAPSY-UHFFFAOYSA-N
Formula: C17H26O10
SMILES: CCCCOC1OC(C(=O)OC)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 390.38

Physical Properties

Property code	Value	Unit	Source
gf	-1040.93	kJ/mol	Joback Method
hf	-1664.67	kJ/mol	Joback Method
hfus	56.22	kJ/mol	Joback Method
hvap	96.17	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	0.496		Crippen Method
mcvol	281.030	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	943.76	K	Joback Method
tc	1158.76	K	Joback Method
tf	609.21	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.04	J/mol×K	943.76	Joback Method
cpg	970.18	J/mol×K	979.59	Joback Method
cpg	980.27	J/mol×K	1015.43	Joback Method
cpg	988.26	J/mol×K	1051.26	Joback Method
cpg	994.08	J/mol×K	1087.10	Joback Method
cpg	997.66	J/mol×K	1122.93	Joback Method
cpg	998.94	J/mol×K	1158.76	Joback Method
dvisc	0.0004311	Pa×s	609.21	Joback Method

dvisc	0.0002905	Pa×s	664.97	Joback Method
dvisc	0.0002081	Pa×s	720.73	Joback Method
dvisc	0.0001564	Pa×s	776.49	Joback Method
dvisc	0.0001221	Pa×s	832.24	Joback Method
dvisc	0.0000984	Pa×s	888.00	Joback Method
dvisc	0.0000813	Pa×s	943.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554419&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