(R)-2-Butyl glucuronide, methyl ester, triacetate

Inchi: InChI=1S/C17H26O10/c1-7-8(2)23-17-15(26-11(5)20)13(25-10(4)19)12(24-9(3)18)14(27
InchiKey: USMXXCSZCGJCAC-SNBXIZFTSA-N
Formula: C17H26O10
SMILES: CCC(C)OC1OC(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	-1043.37	kJ/mol	Joback Method
hf	-1669.95	kJ/mol	Joback Method
hfus	52.70	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.494		Crippen Method
mcvol	281.030	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tb	943.32	K	Joback Method
tc	1159.31	K	Joback Method
tf	594.21	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.52	J/mol×K	943.32	Joback Method
cpg	997.91	J/mol×K	1123.31	Joback Method
cpg	994.43	J/mol×K	1087.31	Joback Method
cpg	988.69	J/mol×K	1051.31	Joback Method
cpg	980.75	J/mol×K	1015.32	Joback Method
cpg	970.67	J/mol×K	979.32	Joback Method
cpg	999.05	J/mol×K	1159.31	Joback Method
dvisc	0.0000741	Pa×s	943.32	Joback Method

dvisc	0.0000908	Pa×s	885.13	Joback Method
dvisc	0.0001143	Pa×s	826.95	Joback Method
dvisc	0.0001491	Pa×s	768.77	Joback Method
dvisc	0.0002032	Pa×s	710.58	Joback Method
dvisc	0.0002926	Pa×s	652.39	Joback Method
dvisc	0.0004525	Pa×s	594.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554697&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