(S)-2-Methylbutyl glucuronide, acetate

Inchi: InChI=1S/C17H26O10/c1-6-8(2)7-23-17-15(26-11(5)20)13(25-10(4)19)12(24-9(3)18)14(2
InchiKey: XVAQZOGXCVYXML-SNBXIZFTSA-N
Formula: C17H26O10
SMILES: CCC(C)COC1OC(C(=O)O)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	-1075.19	kJ/mol	Joback Method
hf	-1689.96	kJ/mol	Joback Method
hfus	55.60	kJ/mol	Joback Method
hvap	110.05	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	0.654		Crippen Method
mcvol	281.030	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook
tb	1013.08	K	Joback Method
tc	1240.35	K	Joback Method
tf	632.80	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.47	J/mol×K	1013.08	Joback Method
cpg	989.36	J/mol×K	1050.96	Joback Method
cpg	995.99	J/mol×K	1088.84	Joback Method
cpg	1000.30	J/mol×K	1126.72	Joback Method
cpg	1002.24	J/mol×K	1164.60	Joback Method
cpg	1001.76	J/mol×K	1202.48	Joback Method
cpg	998.80	J/mol×K	1240.35	Joback Method
dvisc	0.0001795	Pa×s	632.80	Joback Method

dvisc	0.0000939	Pa×s	696.18	Joback Method
dvisc	0.0000548	Pa×s	759.56	Joback Method
dvisc	0.0000347	Pa×s	822.94	Joback Method
dvisc	0.0000235	Pa×s	886.32	Joback Method
dvisc	0.0000167	Pa×s	949.70	Joback Method
dvisc	0.0000124	Pa×s	1013.08	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=R554766&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