Isopentyl glucuronide, methyl ester, triacetate

Inchi: InChI=1S/C18H28O10/c1-9(2)7-8-24-18-16(27-12(5)21)14(26-11(4)20)13(25-10(3)19)15
InchiKey: QJLSBRRINCGZRM-UHFFFAOYSA-N
Formula: C18H28O10
SMILES: COC(=O)C1OC(OCCC(C)C)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 404.41

Physical Properties

Property code	Value	Unit	Source
gf	-1034.95	kJ/mol	Joback Method
hf	-1690.59	kJ/mol	Joback Method
hfus	55.29	kJ/mol	Joback Method
hvap	98.01	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	0.742		Crippen Method
mcvol	295.120	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	2095.00		NIST Webbook
tb	966.20	K	Joback Method
tc	1184.88	K	Joback Method
tf	605.48	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.31	J/mol×K	966.20	Joback Method
cpg	1029.09	J/mol×K	1002.65	Joback Method
cpg	1038.66	J/mol×K	1039.09	Joback Method
cpg	1045.95	J/mol×K	1075.54	Joback Method
cpg	1050.89	J/mol×K	1111.98	Joback Method
cpg	1053.42	J/mol×K	1148.43	Joback Method
cpg	1053.48	J/mol×K	1184.88	Joback Method
dvisc	0.0004098	Pa×s	605.48	Joback Method
dvisc	0.0002620	Pa×s	665.60	Joback Method

dvisc	0.0001804	Pa×s	725.72	Joback Method
dvisc	0.0001315	Pa×s	785.84	Joback Method
dvisc	0.0001003	Pa×s	845.96	Joback Method
dvisc	0.0000792	Pa×s	906.08	Joback Method
dvisc	0.0000645	Pa×s	966.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554533&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