

Isopropyl glucuronide, methyl ester, triacetate

Inchi:	InChI=1S/C16H24O10/c1-7(2)22-16-14(25-10(5)19)12(24-9(4)18)11(23-8(3)17)13(26-16
InchiKey:	WMLVFLHCFASTLY-UHFFFAOYSA-N
Formula:	C16H24O10
SMILES:	<chem>COC(=O)C1OC(OC(C)C)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O</chem>
Mol. weight [g/mol]:	376.36

Physical Properties

Property code	Value	Unit	Source
gf	-1051.79	kJ/mol	Joback Method
hf	-1649.31	kJ/mol	Joback Method
hfus	50.11	kJ/mol	Joback Method
hvap	93.56	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	0.104		Crippen Method
mcvol	266.940	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
rinpol	1910.00		NIST Webbook
tb	920.44	K	Joback Method
tc	1134.63	K	Joback Method
tf	582.94	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.02	J/molxK	920.44	Joback Method
cpg	942.22	J/molxK	1098.93	Joback Method
cpg	937.94	J/molxK	1063.23	Joback Method
cpg	931.51	J/molxK	1027.53	Joback Method
cpg	923.00	J/molxK	991.84	Joback Method
cpg	912.49	J/molxK	956.14	Joback Method
cpg	944.29	J/molxK	1134.63	Joback Method
dvisc	0.0000850	Paxs	920.44	Joback Method
dvisc	0.0001037	Paxs	864.19	Joback Method

dvisc	0.0001300	Paxs	807.94	Joback Method
dvisc	0.0001687	Paxs	751.69	Joback Method
dvisc	0.0002282	Paxs	695.44	Joback Method
dvisc	0.0003257	Paxs	639.19	Joback Method
dvisc	0.0004978	Paxs	582.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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