

Isopentyl glucuronide, acetate

Inchi:	InChI=1S/C17H26O10/c1-8(2)6-7-23-17-15(26-11(5)20)13(25-10(4)19)12(24-9(3)18)14(2
InchiKey:	SNRAFAUYYZLVHY-UHFFFAOYSA-N
Formula:	C17H26O10
SMILES:	CC(=O)OC1C(OCCC(C)C)OC(C(=O)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
rinsol	2010.00		NIST Webbook
tb	1013.08	K	Joback Method
tc	1240.35	K	Joback Method
tf	632.80	K	Joback Method
vc	1.046	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.47	J/molxK	1013.08	Joback Method
cpg	1001.76	J/molxK	1202.48	Joback Method
cpg	1002.24	J/molxK	1164.60	Joback Method
cpg	1000.30	J/molxK	1126.72	Joback Method
cpg	995.99	J/molxK	1088.84	Joback Method
cpg	989.36	J/molxK	1050.96	Joback Method
cpg	998.80	J/molxK	1240.35	Joback Method
dvisc	0.0000124	Paxs	1013.08	Joback Method
dvisc	0.0000167	Paxs	949.70	Joback Method

dvisc	0.0000235	Paxs	886.32	Joback Method
dvisc	0.0000347	Paxs	822.94	Joback Method
dvisc	0.0000548	Paxs	759.56	Joback Method
dvisc	0.0000939	Paxs	696.18	Joback Method
dvisc	0.0001795	Paxs	632.80	Joback Method

Sources

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=R554528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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