

Propyl glucuronide, acetate

Inchi:	InChI=1S/C15H22O10/c1-5-6-21-15-13(24-9(4)18)11(23-8(3)17)10(22-7(2)16)12(25-15)
InchiKey:	ULFDAGPSLQIKGA-UHFFFAOYSA-N
Formula:	C15H22O10
SMILES:	CCCOC1OC(C(=O)O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	362.33

Physical Properties

Property code	Value	Unit	Source
gf	-1089.59	kJ/mol	Joback Method
hf	-1643.40	kJ/mol	Joback Method
hfus	53.94	kJ/mol	Joback Method
hvap	105.99	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	0.018		Crippen Method
mvol	252.850	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	967.76	K	Joback Method
tc	1185.66	K	Joback Method
tf	625.26	K	Joback Method
vc	0.941	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.62	J/molxK	967.76	Joback Method
cpg	874.15	J/molxK	1004.08	Joback Method
cpg	881.76	J/molxK	1040.39	Joback Method
cpg	887.42	J/molxK	1076.71	Joback Method
cpg	891.07	J/molxK	1113.03	Joback Method
cpg	892.64	J/molxK	1149.34	Joback Method
cpg	892.09	J/molxK	1185.66	Joback Method
dvisc	0.0002152	Paxs	625.26	Joback Method

dvisc	0.0001215	Paxs	682.34	Joback Method
dvisc	0.0000749	Paxs	739.43	Joback Method
dvisc	0.0000495	Paxs	796.51	Joback Method
dvisc	0.0000345	Paxs	853.59	Joback Method
dvisc	0.0000252	Paxs	910.68	Joback Method
dvisc	0.0000191	Paxs	967.76	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=R554642&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
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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