

(S)-2-Butyl glucuronide, acetate

Inchi:	InChI=1S/C16H24O10/c1-6-7(2)22-16-14(25-10(5)19)12(24-9(4)18)11(23-8(3)17)13(26-
InchiKey:	XEHILUYIXVGVPR-JPWIBZRCSA-N
Formula:	C16H24O10
SMILES:	CCC(C)OC1OC(C(=O)O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	376.36

Physical Properties

Property code	Value	Unit	Source
gf	-1083.61	kJ/mol	Joback Method
hf	-1669.32	kJ/mol	Joback Method
hfus	53.01	kJ/mol	Joback Method
hvap	107.83	kJ/mol	Joback Method
log10ws	-1.44		Crippen Method
logp	0.406		Crippen Method
mvol	266.940	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1906.00		NIST Webbook
rinpol	1906.00		NIST Webbook
tb	990.20	K	Joback Method
tc	1212.52	K	Joback Method
tf	621.53	K	Joback Method
vc	0.991	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.66	J/molxK	990.20	Joback Method
cpg	931.89	J/molxK	1027.25	Joback Method
cpg	939.03	J/molxK	1064.31	Joback Method
cpg	944.04	J/molxK	1101.36	Joback Method
cpg	946.86	J/molxK	1138.41	Joback Method
cpg	947.43	J/molxK	1175.47	Joback Method
cpg	945.70	J/molxK	1212.52	Joback Method
dvisc	0.0002065	Paxs	621.53	Joback Method

dvisc	0.0001091	Paxs	682.98	Joback Method
dvisc	0.0000640	Paxs	744.42	Joback Method
dvisc	0.0000408	Paxs	805.87	Joback Method
dvisc	0.0000277	Paxs	867.31	Joback Method
dvisc	0.0000198	Paxs	928.76	Joback Method
dvisc	0.0000147	Paxs	990.20	Joback Method

Sources

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=R554726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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