

(S)-2-Butyl glucuronide, methyl ester, triacetate

Inchi:	InChI=1S/C17H26O10/c1-7-8(2)23-17-15(26-11(5)20)13(25-10(4)19)12(24-9(3)18)14(27
InchiKey:	USMXXCSZCGJCAC-HWFFVQPHASA-N
Formula:	C17H26O10
SMILES:	CCC(C)OC1OC(C(=O)OC)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	390.38

Physical Properties

Property code	Value	Unit	Source
gf	-1043.37	kJ/mol	Joback Method
hf	-1669.95	kJ/mol	Joback Method
hfus	52.70	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.494		Crippen Method
mcvol	281.030	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinsol	2000.00		NIST Webbook
tb	943.32	K	Joback Method
tc	1159.31	K	Joback Method
tf	594.21	K	Joback Method
vc	1.046	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.52	J/molxK	943.32	Joback Method
cpg	997.91	J/molxK	1123.31	Joback Method
cpg	994.43	J/molxK	1087.31	Joback Method
cpg	988.69	J/molxK	1051.31	Joback Method
cpg	980.75	J/molxK	1015.32	Joback Method
cpg	970.67	J/molxK	979.32	Joback Method
cpg	999.05	J/molxK	1159.31	Joback Method
dvisc	0.0000741	Paxs	943.32	Joback Method
dvisc	0.0000908	Paxs	885.13	Joback Method

dvisc	0.0001143	Paxs	826.95	Joback Method
dvisc	0.0001491	Paxs	768.77	Joback Method
dvisc	0.0002032	Paxs	710.58	Joback Method
dvisc	0.0002926	Paxs	652.39	Joback Method
dvisc	0.0004525	Paxs	594.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554731&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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