

Butyl citrate

Other names:

1,2,3-Propanetricarboxylic acid, 2-hydroxy-, tributyl ester
Citric acid, tributyl ester
n-Butyl citrate
Citroflex 4
Tri-n-butyl citrate
Tributyl citrate
2-Hydroxy-1,2,3-propanetricarboxylic acid, tributyl ester
Citric acid tri-n-butyl ester
1,2,3-Propanetricarboxylic acid, 2-hydroxy-, 1,2,3-tributyl ester
NSC 8491

Inchi:

InChI=1S/C18H32O7/c1-4-7-10-23-15(19)13-18(22,17(21)25-12-9-6-3)14-16(20)24-11-8

InchiKey:

ZFOZVQLOBQUTQQ-UHFFFAOYSA-N

Formula:

C18H32O7

SMILES:

CCCCOC(=O)CC(O)(CC(=O)OCCCC)C(=O)OCCCC

Mol. weight [g/mol]:

360.44

CAS:

77-94-1

Physical Properties

Property code	Value	Unit	Source
gf	-735.06	kJ/mol	Joback Method
hf	-1310.23	kJ/mol	Joback Method
hfus	47.41	kJ/mol	Joback Method
hvap	98.51	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.528		Crippen Method
mcvol	292.670	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	929.06	K	Joback Method
tc	1137.66	K	Joback Method
tf	572.34	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.86	J/molxK	929.06	Joback Method
cpg	977.62	J/molxK	963.83	Joback Method
cpg	990.18	J/molxK	998.59	Joback Method
cpg	1001.55	J/molxK	1033.36	Joback Method
cpg	1011.76	J/molxK	1068.13	Joback Method
cpg	1020.84	J/molxK	1102.89	Joback Method
cpg	1028.80	J/molxK	1137.66	Joback Method
dvisc	0.0001569	Paxs	572.34	Joback Method
dvisc	0.0000682	Paxs	631.79	Joback Method
dvisc	0.0000342	Paxs	691.25	Joback Method
dvisc	0.0000191	Paxs	750.70	Joback Method
dvisc	0.0000116	Paxs	810.15	Joback Method
dvisc	0.0000076	Paxs	869.61	Joback Method
dvisc	0.0000052	Paxs	929.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77941&Units=SI

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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