

Tributyl acetylcitrate

Other names:	1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tributyl ester Citric acid, tributyl ester, acetate Blo-trol Citroflex A Citroflex A 4 Tributyl acetylcitrate Tributyl citrate acetate Tributyl O-acetylcitrate Tributyl 2-(acetyloxy)-1,2,3-propanetricarboxylic acid Tributyl 2-acetoxy-1,2,3-propanetricarboxylate 2-Acetoxy-1,2,3-propanetricarboxylic acid tributyl ester Acetyl tributyl citrate 2-(Acetyloxy)-1,2,3-propane tricarboxylic acid, tributyl ester Acetyl butyl citrate Acetyl tri-n-butyl citrate Acetylcitric acid, tributyl ester Estaflex ATC O-Acetylcitric acid tributyl ester Tributyl 2-(acetyloxy)-1,2,3-propanetricarboxylate Uniplex 84 1,2,3-Propanetricarboxylic acid, 2-acetoxy-, tributyl ester 1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, 1,2,3-tributyl ester NSC 3894
Inchi:	InChI=1S/C20H34O8/c1-5-8-11-25-17(22)14-20(28-16(4)21,19(24)27-13-10-7-3)15-18(2)
InchiKey:	QZCLKYGREBVARF-UHFFFAOYSA-N
Formula:	C20H34O8
SMILES:	CCCCOC(=O)CC(CC(=O)OCCCC)(OC(C)=O)C(=O)OCCCC
Mol. weight [g/mol]:	402.48
CAS:	77-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-815.32	kJ/mol	Joback Method
hf	-1444.08	kJ/mol	Joback Method
hfs	-1848.00	kJ/mol	NIST Webbook
hfus	51.29	kJ/mol	Joback Method

hvap	95.44	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.098		Crippen Method
mcvol	322.420	ml/mol	McGowan Method
pc	1160.87	kPa	Joback Method
rinpol	2253.00		NIST Webbook
rinpol	2254.00		NIST Webbook
rinpol	2253.00		NIST Webbook
rinpol	2253.00		NIST Webbook
rinpol	2224.00		NIST Webbook
rinpol	2253.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	958.93	K	Joback Method
tc	1174.08	K	Joback Method
tf	606.22	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.89	J/molxK	958.93	Joback Method
cpg	1121.42	J/molxK	1138.23	Joback Method
cpg	1113.49	J/molxK	1102.37	Joback Method
cpg	1104.08	J/molxK	1066.51	Joback Method
cpg	1093.19	J/molxK	1030.65	Joback Method
cpg	1080.80	J/molxK	994.79	Joback Method
cpg	1127.88	J/molxK	1174.08	Joback Method
dvisc	0.0000198	Paxs	958.93	Joback Method
dvisc	0.0000258	Paxs	900.14	Joback Method
dvisc	0.0000349	Paxs	841.36	Joback Method
dvisc	0.0000495	Paxs	782.58	Joback Method
dvisc	0.0000743	Paxs	723.79	Joback Method
dvisc	0.0001197	Paxs	665.00	Joback Method
dvisc	0.0002116	Paxs	606.22	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	446.00	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
hfs:	Solid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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