

Batilol

Other names:

dl-Batyl alcohol
Bathyl alcohol
Batyl alcohol
1,2-Propanediol, 3-(octadecyloxy)-
«alpha»-Octadecylether of glycerol
C18:0 Glyceryl 1-ether
Glycerol monoctadecyl ether
Glycerol 1-octadecyl ether
Glyceryl-1-octadecyl ether
Stearyl monoglyceride
1-(Octadecyloxy)-2,3-dihydroxypropane
1-O-Octadecylglycerol
3-(Octadecyloxy)-1,2-propanediol
Glycerine 1-monostearyl ether
Monoctadecyl ether of glycerol
Batylol
NSC 284200
Batil alcohol

Inchi:

InChI=1S/C21H44O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-24-20-21(23)19-22

InchiKey:

OGBUMNBNEWYMNJ-UHFFFAOYSA-N

Formula:

C21H44O3

SMILES:

CCCCCCCCCCCCCCCCCCOCC(O)CO

Mol. weight [g/mol]:

344.57

CAS:

544-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-255.14	kJ/mol	Joback Method
hf	-918.73	kJ/mol	Joback Method
hfus	55.99	kJ/mol	Joback Method
hvap	97.72	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.618		Crippen Method
mcvol	324.360	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	2608.70		NIST Webbook
rinpol	2608.70		NIST Webbook

tb	886.22	K	Joback Method
tc	1091.93	K	Joback Method
tf	455.30	K	Joback Method
vc	1.262	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.75	J/mol×K	886.22	Joback Method
cpg	1118.31	J/mol×K	920.51	Joback Method
cpg	1136.67	J/mol×K	954.79	Joback Method
cpg	1153.87	J/mol×K	989.08	Joback Method
cpg	1169.97	J/mol×K	1023.36	Joback Method
cpg	1185.02	J/mol×K	1057.65	Joback Method
cpg	1199.06	J/mol×K	1091.93	Joback Method
dvisc	0.0007152	Paxs	455.30	Joback Method
dvisc	0.0001228	Paxs	527.12	Joback Method
dvisc	0.0000322	Paxs	598.94	Joback Method
dvisc	0.0000112	Paxs	670.76	Joback Method
dvisc	0.0000048	Paxs	742.58	Joback Method
dvisc	0.0000024	Paxs	814.40	Joback Method
dvisc	0.0000013	Paxs	886.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544627&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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