Butanedioic acid, 2,3-dihydroxy-, dibutyl ester

Inchi: InChI=1S/C12H22O6/c1-3-5-7-17-11(15)9(13)10(14)12(16)18-8-6-4-2/h9-10,13-14H,3-8H
InchiKey: PCYQQSKDZQTOQG-UHFFFAOYSA-N
Formula: C12H22O6
SMILES: CCCCOC(=O)C(O)C(O)C(=O)OCCCC
Mol. weight [g/mol]: 262.30
CAS: 344268-32-2

Physical Properties

Property code	Value	Unit	Source
gf	-696.20	kJ/mol	Joback Method
hf	-1095.63	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	93.20	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.395		Crippen Method
mcvol	206.560	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	810.02	K	Joback Method
tc	994.77	K	Joback Method
tf	460.96	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.71	J/mol×K	810.02	Joback Method
cpg	644.99	J/mol×K	840.81	Joback Method
cpg	655.54	J/mol×K	871.60	Joback Method
cpg	665.38	J/mol×K	902.40	Joback Method
cpg	674.51	J/mol×K	933.19	Joback Method
cpg	682.92	J/mol×K	963.98	Joback Method
cpg	690.64	J/mol×K	994.77	Joback Method
dvisc	0.0008016	Pa×s	460.96	Joback Method
dvisc	0.0002009	Pa×s	519.14	Joback Method

dvisc	0.0000666	Pa×s	577.31	Joback Method
dvisc	0.0000270	Pa×s	635.49	Joback Method
dvisc	0.0000127	Pa×s	693.67	Joback Method
dvisc	0.0000067	Pa×s	751.84	Joback Method
dvisc	0.0000039	Pa×s	810.02	Joback Method

Sources

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=C344268322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume