Ethylene glycol di-n-butyrate

Other names: Butanoic acid, 1,2-ethanediyl ester
Inchi: InChI=1S/C10H18O4/c1-3-5-9(11)13-7-8-14-10(12)6-4-2/h3-8H2,1-2H3
InchiKey: SFTRWCBAYKQWCS-UHFFFAOYSA-N
Formula: C10H18O4
SMILES: CCCC(=O)OCCOC(=O)CCC
Mol. weight [g/mol]: 202.25
CAS: 105-72-6

Physical Properties

Property code	Value	Unit	Source
gf	-434.52	kJ/mol	Joback Method
hf	-739.33	kJ/mol	Joback Method
hfus	27.23	kJ/mol	Joback Method
hvap	73.21 ± 0.60	kJ/mol	NIST Webbook
hvap	73.20 ± 0.60	kJ/mol	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.673		Crippen Method
mcvol	166.640	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
tb	580.78	K	Joback Method
tc	760.87	K	Joback Method
tf	346.78	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.69	J/mol×K	580.78	Joback Method
cpg	428.88	J/mol×K	610.80	Joback Method
cpg	441.54	J/mol×K	640.81	Joback Method
cpg	453.66	J/mol×K	670.83	Joback Method
cpg	465.23	J/mol×K	700.84	Joback Method
cpg	476.26	J/mol×K	730.86	Joback Method
cpg	486.74	J/mol×K	760.87	Joback Method

cpl	380.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0019074	Pa×s	346.78	Joback Method
dvisc	0.0010682	Pa×s	385.78	Joback Method
dvisc	0.0006655	Pa×s	424.78	Joback Method
dvisc	0.0004489	Pa×s	463.78	Joback Method
dvisc	0.0003219	Pa×s	502.78	Joback Method
dvisc	0.0002421	Pa×s	541.78	Joback Method
dvisc	0.0001892	Pa×s	580.78	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=C105726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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

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