Butanedioic acid, ethyl-(2-methyl-1-butyl) ester

Inchi: InChI=1S/C11H20O4/c1-4-9(3)8-15-11(13)7-6-10(12)14-5-2/h9H,4-8H2,1-3H3
InchiKey: ODJKTHLKSYNUAD-UHFFFAOYSA-N
Formula: C11H20O4
SMILES: CCOC(=O)CCC(=O)OCC(C)CC
Mol. weight [g/mol]: 216.27

Physical Properties

Property code	Value	Unit	Source
gf	-428.54	kJ/mol	Joback Method
hf	-765.25	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.919		Crippen Method
mcvol	180.730	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1424.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1424.00		NIST Webbook
tb	603.22	K	Joback Method
tc	784.89	K	Joback Method
tf	343.05	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.43	J/mol×K	603.22	Joback Method
cpg	479.63	J/mol×K	633.50	Joback Method
cpg	493.21	J/mol×K	663.78	Joback Method
cpg	506.18	J/mol×K	694.06	Joback Method
cpg	518.53	J/mol×K	724.34	Joback Method
cpg	530.27	J/mol×K	754.61	Joback Method
cpg	541.38	J/mol×K	784.89	Joback Method

dvisc	0.0022861	Pa×s	343.05	Joback Method
dvisc	0.0011425	Pa×s	386.41	Joback Method
dvisc	0.0006567	Pa×s	429.77	Joback Method
dvisc	0.0004178	Pa×s	473.13	Joback Method
dvisc	0.0002868	Pa×s	516.50	Joback Method
dvisc	0.0002087	Pa×s	559.86	Joback Method
dvisc	0.0001589	Pa×s	603.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R106793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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