Dimethylmalonic acid, butyl isobutyl ester

Inchi: InChI=1S/C13H24O4/c1-6-7-8-16-11(14)13(4,5)12(15)17-9-10(2)3/h10H,6-9H2,1-5H3
InchiKey: MZTUUMXZESEQDF-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CCCCOC(=O)C(C)(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
gf	-408.86	kJ/mol	Joback Method
hf	-815.28	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	61.16	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.555		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	1420.00		NIST Webbook
tb	645.75	K	Joback Method
tc	832.89	K	Joback Method
tf	368.01	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.62	J/mol×K	645.75	Joback Method
cpg	587.54	J/mol×K	676.94	Joback Method
cpg	602.64	J/mol×K	708.13	Joback Method
cpg	616.93	J/mol×K	739.32	Joback Method
cpg	630.43	J/mol×K	770.51	Joback Method
cpg	643.16	J/mol×K	801.70	Joback Method
cpg	655.14	J/mol×K	832.89	Joback Method
dvisc	0.0021445	Pa×s	368.01	Joback Method
dvisc	0.0009889	Pa×s	414.30	Joback Method

dvisc	0.0005328	Pa×s	460.59	Joback Method
dvisc	0.0003214	Pa×s	506.88	Joback Method
dvisc	0.0002110	Pa×s	553.17	Joback Method
dvisc	0.0001478	Pa×s	599.46	Joback Method
dvisc	0.0001090	Pa×s	645.75	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361651&Units=SI

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