Butanedioic acid, ethyl-(1-methylethyl) ester

Inchi: InChI=1S/C9H16O4/c1-4-12-8(10)5-6-9(11)13-7(2)3/h7H,4-6H2,1-3H3
InchiKey: VPEYKSOKDHUUJO-UHFFFAOYSA-N
Formula: C9H16O4
SMILES: CCOC(=O)CCC(=O)OC(C)C
Mol. weight [g/mol]: 188.22

Physical Properties

Property code	Value	Unit	Source
gf	-445.38	kJ/mol	Joback Method
hf	-723.97	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.281		Crippen Method
mcvol	152.550	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1325.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
tb	557.46	K	Joback Method
tc	742.78	K	Joback Method
tf	320.51	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.40	J/mol×K	557.46	Joback Method
cpg	381.08	J/mol×K	588.35	Joback Method
cpg	393.25	J/mol×K	619.23	Joback Method
cpg	404.90	J/mol×K	650.12	Joback Method
cpg	416.03	J/mol×K	681.01	Joback Method
cpg	426.64	J/mol×K	711.90	Joback Method
cpg	436.72	J/mol×K	742.78	Joback Method

dvisc	0.0025423	Pa×s	320.51	Joback Method
dvisc	0.0013123	Pa×s	360.00	Joback Method
dvisc	0.0007719	Pa×s	399.49	Joback Method
dvisc	0.0004996	Pa×s	438.99	Joback Method
dvisc	0.0003474	Pa×s	478.48	Joback Method
dvisc	0.0002553	Pa×s	517.97	Joback Method
dvisc	0.0001960	Pa×s	557.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R106788&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume