Butanoic acid, 2,2-diethyl-3,3-dimethyl, ethyl ester

Inchi: InChI=1S/C12H24O2/c1-7-12(8-2,11(4,5)6)10(13)14-9-3/h7-9H2,1-6H3
InchiKey: PDIVLKNUSLZXIC-UHFFFAOYSA-N
Formula: C12H24O2
SMILES: CCOC(=O)C(CC)(CC)C(C)(C)C
Mol. weight [g/mol]: 200.32

Physical Properties

Property code	Value	Unit	Source
gf	-178.08	kJ/mol	Joback Method
hf	-553.31	kJ/mol	Joback Method
hfus	14.79	kJ/mol	Joback Method
hvap	48.87	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.402		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	1248.00		NIST Webbook
tb	543.79	K	Joback Method
tc	732.60	K	Joback Method
tf	302.00	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.94	J/mol×K	543.79	Joback Method
cpg	487.55	J/mol×K	575.26	Joback Method
cpg	504.22	J/mol×K	606.73	Joback Method
cpg	519.99	J/mol×K	638.19	Joback Method
cpg	534.88	J/mol×K	669.66	Joback Method
cpg	548.95	J/mol×K	701.13	Joback Method
cpg	562.23	J/mol×K	732.60	Joback Method
dvisc	0.0047329	Pa×s	302.00	Joback Method
dvisc	0.0019385	Pa×s	342.30	Joback Method

dvisc	0.0009583	Pa×s	382.60	Joback Method
dvisc	0.0005418	Pa×s	422.89	Joback Method
dvisc	0.0003382	Pa×s	463.19	Joback Method
dvisc	0.0002277	Pa×s	503.49	Joback Method
dvisc	0.0001626	Pa×s	543.79	Joback Method

Sources

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=R108175&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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