Butanoic acid, 2-ethyl-2,3,3-trimethyl, ethyl ester

Inchi: InChI=1S/C11H22O2/c1-7-11(6,10(3,4)5)9(12)13-8-2/h7-8H2,1-6H3
InchiKey: LAFWOZVYMOJZBC-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCOC(=O)C(C)(CC)C(C)(C)C
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-186.50	kJ/mol	Joback Method
hf	-532.67	kJ/mol	Joback Method
hfus	12.21	kJ/mol	Joback Method
hvap	46.64	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.012		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1146.00		NIST Webbook
rinpol	1146.00		NIST Webbook
tb	520.91	K	Joback Method
tc	712.01	K	Joback Method
tf	290.73	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.01	J/mol×K	520.91	Joback Method
cpg	438.07	J/mol×K	552.76	Joback Method
cpg	454.19	J/mol×K	584.61	Joback Method
cpg	469.43	J/mol×K	616.46	Joback Method
cpg	483.81	J/mol×K	648.31	Joback Method
cpg	497.38	J/mol×K	680.16	Joback Method
cpg	510.18	J/mol×K	712.01	Joback Method
dvisc	0.0052121	Pa×s	290.73	Joback Method

dvisc	0.0021611	Pa×s	329.09	Joback Method
dvisc	0.0010769	Pa×s	367.46	Joback Method
dvisc	0.0006122	Pa×s	405.82	Joback Method
dvisc	0.0003837	Pa×s	444.18	Joback Method
dvisc	0.0002590	Pa×s	482.55	Joback Method
dvisc	0.0001852	Pa×s	520.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R108219&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