

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

Inchi:	InChI=1S/C9H18O2/c1-5-8(7(3)4)9(10)11-6-2/h7-8H,5-6H2,1-4H3
InchiKey:	LQQJUPMYOFCSCR-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCOC(=O)C(CC)C(C)C
Mol. weight [g/mol]:	158.24

Physical Properties

Property code	Value	Unit	Source
gf	-213.90	kJ/mol	Joback Method
hf	-484.45	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	2.232		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	983.00		NIST Webbook
tb	480.73	K	Joback Method
tc	661.81	K	Joback Method
tf	233.35	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.22	J/molxK	480.73	Joback Method
cpg	387.73	J/molxK	631.63	Joback Method
cpg	375.88	J/molxK	601.45	Joback Method
cpg	363.51	J/molxK	571.27	Joback Method
cpg	350.61	J/molxK	541.09	Joback Method
cpg	337.19	J/molxK	510.91	Joback Method
cpg	399.06	J/molxK	661.81	Joback Method
dvisc	0.0002156	Paxs	480.73	Joback Method
dvisc	0.0002948	Paxs	439.50	Joback Method

dvisc	0.0004299	Paxs	398.27	Joback Method
dvisc	0.0006840	Paxs	357.04	Joback Method
dvisc	0.0012286	Paxs	315.81	Joback Method
dvisc	0.0026314	Paxs	274.58	Joback Method
dvisc	0.0073761	Paxs	233.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R108244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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

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