

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

Other names:	Butyric acid, 2-ethyl-2-methyl-, methyl ester Methyl «alpha»-ethyl-«alpha»-methylbutyrate Methyl «alpha»-methyl-«alpha»-ethylbutyrate
Inchi:	InChI=1S/C8H16O2/c1-5-8(3,6-2)7(9)10-4/h5-6H2,1-4H3
InchiKey:	RUFXPLNQCKJCCF-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCC(C)(CC)C(=O)OC
Mol. weight [g/mol]:	144.21
CAS:	5296-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-214.60	kJ/mol	Joback Method
hf	-462.00	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	41.26	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	869.00		NIST Webbook
rinpol	869.00		NIST Webbook
tb	455.50	K	Joback Method
tc	641.54	K	Joback Method
tf	254.50	K	Joback Method
vc	0.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.32	J/mol×K	455.50	Joback Method
cpg	295.73	J/mol×K	486.51	Joback Method
cpg	308.53	J/mol×K	517.51	Joback Method
cpg	320.73	J/mol×K	548.52	Joback Method

cpg	332.35	J/molxK	579.53	Joback Method
cpg	343.41	J/molxK	610.54	Joback Method
cpg	353.92	J/molxK	641.54	Joback Method
dvisc	0.0046923	Paxs	254.50	Joback Method
dvisc	0.0021847	Paxs	288.00	Joback Method
dvisc	0.0011929	Paxs	321.50	Joback Method
dvisc	0.0007301	Paxs	355.00	Joback Method
dvisc	0.0004864	Paxs	388.50	Joback Method
dvisc	0.0003456	Paxs	422.00	Joback Method
dvisc	0.0002582	Paxs	455.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5296708&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
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

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