Butanoic acid, 2-methyl-, 2-methylbutyl ester

Other names:	Butyric acid, 2-methyl-, 2-methylbutyl ester
	2-Methylbutyl 2-methylbutanoate
	2-Methylbutyl 2-methylbutyrate
	dl-2-Methylbutyric acid 2-methylbutyl ester
	2-Methylbutanoic acid 2-methylbutyl ester
	2-Methyl buthyl 2-methyl butanoate
Inchi:	InChI=1S/C10H20O2/c1-5-8(3)7-12-10(11)9(4)6-2/h8-9H,5-7H2,1-4H3
InchiKey:	PVYFCGRBIREQLL-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCC(C)COC(=O)C(C)CC
Mol. weight [g/mol]:	172.26
CAS:	2445-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-205.48	kJ/mol	Joback Method
hf	-505.09	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1104.40		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1102.00		NIST Webbook

rinpol	1106.10		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1107.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1274.00		NIST Webbook
ripol	1282.00		NIST Webbook
ripol	1277.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1276.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1284.00		NIST Webbook
ripol	1283.00		NIST Webbook
ripol	1279.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1292.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1286.00		NIST Webbook
tb	503.61	K	Joback Method
tc	682.96	K	Joback Method
tf	244.62	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	368.51	J/mol×K	503.61	Joback Method
cpg	383.39	J/mol×K	533.50	Joback Method
cpg	397.67	J/mol×K	563.39	Joback Method
cpg	411.38	J/mol×K	593.28	Joback Method
cpg	424.51	J/mol×K	623.18	Joback Method
cpg	437.08	J/mol×K	653.07	Joback Method
cpg	449.08	J/mol×K	682.96	Joback Method
dvisc	0.0070487	Pa×s	244.62	Joback Method
dvisc	0.0024917	Pa×s	287.79	Joback Method
dvisc	0.0011553	Pa×s	330.95	Joback Method
dvisc	0.0006396	Pa×s	374.12	Joback Method
dvisc	0.0004002	Pa×s	417.28	Joback Method
dvisc	0.0002734	Pa×s	460.44	Joback Method
dvisc	0.0001994	Pa×s	503.61	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=C2445785&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume