

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

Other names:	2-Methylbutyl 3-methylbutanoate 2-Methylbutyl 3-methylbutyrate 2-Methylbutyl isopentanoate 2-Methylbutyl isovalerate 2-methylbutyl isovalerate (2-methylbutyl-3-methyl butyrate) Isovaleric acid, 2-methylbutyl ester
Inchi:	InChI=1S/C10H20O2/c1-5-9(4)7-12-10(11)6-8(2)3/h8-9H,5-7H2,1-4H3
InchiKey:	CYGPPWVXOWCHJB-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCC(C)COC(=O)CC(C)C
Mol. weight [g/mol]:	172.26
CAS:	2445-77-4

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	1089.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1108.70		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1113.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1110.20		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1109.00		NIST Webbook

ripol	1110.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1107.00		NIST Webbook
ripol	1299.00		NIST Webbook
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ripol	1299.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1286.00		NIST Webbook
ripol	1295.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1299.00		NIST Webbook
tb	503.61	K	Joback Method
tc	682.96	K	Joback Method
tf	244.62	K	Joback Method
vc	0.608	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.51	J/molxK	503.61	Joback Method
cpg	437.08	J/molxK	653.07	Joback Method
cpg	424.51	J/molxK	623.18	Joback Method
cpg	411.38	J/molxK	593.28	Joback Method
cpg	397.67	J/molxK	563.39	Joback Method
cpg	383.39	J/molxK	533.50	Joback Method
cpg	449.08	J/molxK	682.96	Joback Method
dvisc	0.0001994	Paxs	503.61	Joback Method
dvisc	0.0002734	Paxs	460.44	Joback Method
dvisc	0.0004002	Paxs	417.28	Joback Method
dvisc	0.0006396	Paxs	374.12	Joback Method
dvisc	0.0011553	Paxs	330.95	Joback Method
dvisc	0.0024917	Paxs	287.79	Joback Method
dvisc	0.0070487	Paxs	244.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36327e+01
Coeff. B	-3.67424e+03
Coeff. C	-6.81540e+01
Temperature range (K), min.	343.48
Temperature range (K), max.	509.71

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=C2445774&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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