BUTANOIC ACID, 3-METHYL-, 3-METHYLBUTYL ESTER

Other names: 3-Methylbutyl 3-methylbutyrate
3-Methylbutyl isovalerate
3-methylbutyl 3-methylbutanoate
Apple essence
Apple oil
ISOAMYL ISOVALERATE
Isoamyl 3-methylbutanoate
Isoamyl 3-methylbutyrate
Isoamyl valerianate
Isopentyl 3-methylbutanoate
Isopentyl 3-methylbutyrate
Isopentyl alcohol, isovalerate
Isopentyl isopentanoate
Isopentyl isovalerate
Isovaleric acid, 3-methylbutyl ester
Isovaleric acid, isopentyl ester
NSC 6565
Solusterol
iso-Amyl isovalerate

Inchi: InChI=1S/C10H20O2/c1-8(2)5-6-12-10(11)7-9(3)4/h8-9H,5-7H2,1-4H3

InchiKey: XINCECQTMHSORG-UHFFFAOYSA-N

Formula: C10H20O2

SMILES: CC(C)CCOC(=O)CC(C)C

Mol. weight [g/mol]: 172.27

CAS: 659-70-1

Physical Properties

Property code	Value	Unit	Source
af	0.5531		Cheméo Relay (1.0)
hf	-588.49	kJ/mol	Cheméo Relay (1.0)
hfus	17.40	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method

rinpol	1090.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1090.70	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1110.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1107.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1085.00	NIST Webbook
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ripol	1285.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1294.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1312.00		NIST Webbook
tb	467.15 ± 1.50	K	NIST Webbook
tb	466.70 ± 0.50	K	NIST Webbook
tb	465.85 ± 0.30	K	NIST Webbook
tb	463.60	K	NIST Webbook
tc	637.01	K	Cheméo Relay (1.0)
tf	196.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.08	J/mol×K	682.96	Joback Method
cpg	424.51	J/mol×K	623.18	Joback Method
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	437.08	J/mol×K	653.07	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
hvapt	46.40	kJ/mol	410.00	NIST Webbook
hvapt	47.20	kJ/mol	383.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.97023e+01
Coeff. B	-6.63821e+03
Coeff. C	-3.46649e+00
Coeff. D	1.97306e-06
Temperature range (K), min.	215.00
Temperature range (K), max.	637.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1121
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB: https://www.cheric.org/files/research/kdb/mol/mol1121.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C659701&Units=SI
Cheméo Relay (1.0, beta):
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point