BUTANOIC ACID, 2-METHYL-, HEXYL ESTER

Other names:	Butyric acid, 2-methyl-, hexyl ester
	Hexyl 2-methylbutyrate
	2-Methylbutanoic acid, n-hexyl ester
	n-Hexyl 2-methyl butyrate
	n-Hexyl 2-methylbutanoate
	Hexyl 2-methylbutanoate
Inchi:	InChI=1S/C11H22O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h10H,4-9H2,1-3H3
InchiKey:	YUECNVSODFDKOQ-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCCCOC(=O)C(C)CC
Mol. weight [g/mol]:	186.30

Physical Properties

Property code	Value	Unit	Source
af	0.6116		Cheméo Relay (1.0)
hf	-603.95	kJ/mol	Cheméo Relay (1.0)
hfus	23.51	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-3.42		Cheméo Relay (1.0)
logp	3.156		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1224.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1243.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1228.00		NIST Webbook

rinpol	1240.00	NIST Webbook
rinpol	1237.30	NIST Webbook
rinpol	1204.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1235.00	NIST Webbook
rinpol	1190.00	NIST Webbook
rinpol	1235.00	NIST Webbook
rinpol	1234.00	NIST Webbook
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ripol	1416.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1415.00		NIST Webbook
tb	464.82	K	Cheméo Relay (1.0)
tc	661.24	K	Cheméo Relay (1.0)
tf	210.67	K	Cheméo Relay (1.0)
vc	0.653	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.48	J/mol×K	526.93	Joback Method
cpg	498.48	J/mol×K	701.19	Joback Method
cpg	486.09	J/mol×K	672.15	Joback Method

cpg	473.13	J/mol×K	643.11	Joback Method
cpg	459.60	J/mol×K	614.06	Joback Method
cpg	445.49	J/mol×K	585.02	Joback Method
cpg	430.78	J/mol×K	555.97	Joback Method
dvisc	0.0005632	Pa×s	398.91	Joback Method
dvisc	0.0001937	Pa×s	526.93	Joback Method
dvisc	0.0002597	Pa×s	484.26	Joback Method
dvisc	0.0003684	Pa×s	441.58	Joback Method
dvisc	0.0044896	Pa×s	270.89	Joback Method
dvisc	0.0009531	Pa×s	356.24	Joback Method
dvisc	0.0018616	Pa×s	313.56	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10032152&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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
ie: Ionization energy
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