

Butanoic acid, 1-methylhexyl ester

Other names:	1-Methylhexyl butanoate 2-Heptanol butanoate 2-Heptyl butanoate 2-Heptyl butyrate heptan-2-yl butanoate
Inchi:	InChI=1S/C11H22O2/c1-4-6-7-9-10(3)13-11(12)8-5-2/h10H,4-9H2,1-3H3
InchiKey:	GTKUPJHQSA PWLL-UHFFFAOYSA-N
Formula:	C11H22O2
SMILES:	CCCCC(C)OC(=O)CCC
Mol. weight [g/mol]:	186.29
CAS:	39026-94-3

Physical Properties

Property code	Value	Unit	Source
gf	-194.62	kJ/mol	Joback Method
hf	-520.45	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.298		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1194.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1230.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1396.00		NIST Webbook
tb	526.93	K	Joback Method

tc	701.19	K	Joback Method
tf	270.89	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.48	J/mol×K	526.93	Joback Method
cpg	430.78	J/mol×K	555.97	Joback Method
cpg	445.49	J/mol×K	585.02	Joback Method
cpg	459.60	J/mol×K	614.06	Joback Method
cpg	473.13	J/mol×K	643.11	Joback Method
cpg	486.09	J/mol×K	672.15	Joback Method
cpg	498.48	J/mol×K	701.19	Joback Method
dvisc	0.0044896	Pa×s	270.89	Joback Method
dvisc	0.0018616	Pa×s	313.56	Joback Method
dvisc	0.0009531	Pa×s	356.24	Joback Method
dvisc	0.0005632	Pa×s	398.91	Joback Method
dvisc	0.0003684	Pa×s	441.58	Joback Method
dvisc	0.0002597	Pa×s	484.26	Joback Method
dvisc	0.0001937	Pa×s	526.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47715e+01
Coeff. B	-4.23199e+03
Coeff. C	-7.71340e+01
Temperature range (K), min.	369.32
Temperature range (K), max.	524.49

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39026943&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/ci990307l
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
hvac:	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
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
vc:	Critical Volume

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