

Pentanoic acid, 4-oxo-, butyl ester

Other names:	4-Ketopentanoic acid butyl ester Butyl laevulinate Levulinic acid n-butyl ester Levulinic acid, butyl ester NSC 78451 butyl 4-oxopentanoate butyl 4-oxovalerate butyl levulinate n-Butyl laevulinate n-butyl 4-oxopentanoate n-butyl levulinate
Inchi:	InChI=1S/C9H16O3/c1-3-4-7-12-9(11)6-5-8(2)10/h3-7H2,1-2H3
InchiKey:	ISBWNEKJSSLXOD-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	CCCCOC(=O)CCC(C)=O
Mol. weight [g/mol]:	172.22
CAS:	2052-15-5

Physical Properties

Property code	Value	Unit	Source
gf	-337.94	kJ/mol	Joback Method
hf	-586.47	kJ/mol	Joback Method
hfus	23.45	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.699		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1225.00		NIST Webbook
rinpol	1225.00		NIST Webbook
ripol	1760.00		NIST Webbook
ripol	1760.00		NIST Webbook
tb	510.70	K	NIST Webbook
tc	718.27	K	Joback Method
tf	313.28	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.51	J/molxK	535.48	Joback Method
cpg	356.03	J/molxK	565.94	Joback Method
cpg	368.04	J/molxK	596.41	Joback Method
cpg	379.53	J/molxK	626.87	Joback Method
cpg	390.51	J/molxK	657.34	Joback Method
cpg	400.99	J/molxK	687.80	Joback Method
cpg	410.97	J/molxK	718.27	Joback Method
dvisc	0.0026992	Paxs	313.28	Joback Method
dvisc	0.0014842	Paxs	350.31	Joback Method
dvisc	0.0009150	Paxs	387.35	Joback Method
dvisc	0.0006138	Paxs	424.38	Joback Method
dvisc	0.0004390	Paxs	461.41	Joback Method
dvisc	0.0003300	Paxs	498.45	Joback Method
dvisc	0.0002580	Paxs	535.48	Joback Method
hvapt	56.00	kJ/mol	452.00	NIST Webbook
hvapt	51.00	kJ/mol	446.00	NIST Webbook
hvapt	55.50	kJ/mol	424.50	NIST Webbook
pvap	0.02	kPa	318.00	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	3.93e-03	kPa	298.20	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	6.11e-03	kPa	303.20	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	8.95e-03	kPa	308.10	Renewable platform chemicals: Thermochemical study of levulinic acid esters

pvap	0.01	kPa	313.00	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.18	kPa	347.80	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.13	kPa	342.80	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.09	kPa	337.80	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.06	kPa	332.80	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.04	kPa	327.90	Renewable platform chemicals: Thermochemical study of levulinic acid esters
pvap	0.03	kPa	323.00	Renewable platform chemicals: Thermochemical study of levulinic acid esters
rhol	966.50	kg/m ³	303.15	Solubilities and thermodynamic properties of SO ₂ in five biobased solvents
rhol	969.93	kg/m ³	298.15	Self-aggregation of liquids from biomass in aqueous solution
rhol	975.60	kg/m ³	293.15	Solubilities and thermodynamic properties of SO ₂ in five biobased solvents
rhol	939.80	kg/m ³	333.15	Solubilities and thermodynamic properties of SO ₂ in five biobased solvents

rhoI	949.30	kg/m3	323.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents
rhoI	958.20	kg/m3	313.15	Solubilities and thermodynamic properties of SO2 in five biobased solvents

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	0.80	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Renewable platform chemicals: Thermochemical study of levulinic acid	https://www.doi.org/10.1016/j.tca.2017.12.006
Solubilities of Carbon Dioxide in Five Bio-based Solvents:	https://www.doi.org/10.1021/je500812s
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2052155&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Self-aggregation of liquids from biomass in aqueous solution:	https://www.doi.org/10.1016/j.jct.2013.06.020
Solubilities and thermodynamic properties of SO2 in five biobased solvents:	https://www.doi.org/10.1016/j.jct.2015.09.017

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/92-115-2/Pentanoic-acid-4-oxo-butyl-ester.pdf>

Generated by Cheméo on 2024-04-26 08:55:25.143340291 +0000 UTC m=+16410974.063917603.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.