2,4-Pentanedione, 3-butyl-

Other names:	3-Acetyl-2-heptanone
	3-Butyl-2,4-pentanedione
	3-Butylacetylacetone
	3-Butylpentanedione-2,4
	3-n-Butyl-2,4-pentanedione
	3-butylpentane-2,4-dione
Inchi:	InChI=1S/C9H16O2/c1-4-5-6-9(7(2)10)8(3)11/h9H,4-6H2,1-3H3
InchiKey:	MBXOOYPCIDHXGH-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CCCCC(C(C)=O)C(C)=O
Mol. weight [g/mol]:	156.22
CAS:	1540-36-9

Physical Properties

Property code	Value	Unit	Source
gf	-235.38	kJ/mol	Joback Method
hf	-465.30	kJ/mol	NIST Webbook
hfus	18.74	kJ/mol	Joback Method
hvap	48.73	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.971		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
tb	512.62	K	Joback Method
tc	700.24	K	Joback Method
tf	276.05	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.33	J/mol×K	512.62	Joback Method
cpg	332.39	J/mol×K	543.89	Joback Method
cpg	344.84	J/mol×K	575.16	Joback Method

cpg	356.72	J/mol×K	606.43	Joback Method
cpg	368.02	J/mol×K	637.70	Joback Method
cpg	378.78	J/mol×K	668.97	Joback Method
cpg	388.99	J/mol×K	700.24	Joback Method
dvisc	0.0049787	Pa×s	276.05	Joback Method
dvisc	0.0023185	Pa×s	315.48	Joback Method
dvisc	0.0012795	Pa×s	354.91	Joback Method
dvisc	0.0007952	Pa×s	394.34	Joback Method
dvisc	0.0005389	Pa×s	433.76	Joback Method
dvisc	0.0003896	Pa×s	473.19	Joback Method
dvisc	0.0002961	Pa×s	512.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1540369&Units=SI
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
hvap:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/60-886-2/2-4-Pentanedione-3-butyl.pdf

Generated by Cheméo on 2025-12-05 22:47:42.817504623 +0000 UTC m=+4723060.347545288.

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