2-Ketobutan-3-yl butanoate

Other names: Acetoin butanoate
3-(butanoyloxy)-2-butanone
Inchi: InChI=1S/C8H14O3/c1-4-5-8(10)11-7(3)6(2)9/h7H,4-5H2,1-3H3
InchiKey: LJDWJXUIGKSETE-UHFFFAOYSA-N
Formula: C8H14O3
SMILES: CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 158.19

Physical Properties

Property code	Value	Unit	Source
gf	-348.80	kJ/mol	Joback Method
hf	-571.11	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.307		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1038.00		NIST Webbook
tb	512.16	K	Joback Method
tc	700.78	K	Joback Method
tf	287.01	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.94	J/mol×K	512.16	Joback Method
cpg	310.84	J/mol×K	543.60	Joback Method
cpg	322.24	J/mol×K	575.03	Joback Method
cpg	333.16	J/mol×K	606.47	Joback Method

cpg	343.58	J/mol×K	637.91	Joback Method
cpg	353.52	J/mol×K	669.35	Joback Method
cpg	362.98	J/mol×K	700.78	Joback Method
dvisc	0.0036492	Pa×s	287.01	Joback Method
dvisc	0.0018279	Pa×s	324.53	Joback Method
dvisc	0.0010567	Pa×s	362.06	Joback Method
dvisc	0.0006771	Pa×s	399.58	Joback Method
dvisc	0.0004683	Pa×s	437.11	Joback Method
dvisc	0.0003434	Pa×s	474.63	Joback Method
dvisc	0.0002635	Pa×s	512.16	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R66269&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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