

Butyl glyoxylate

Other names:	Acetic acid, oxo-, butyl ester Butyl glyoxalate Butyl oxoacetate Glyoxylic acid, butyl ester
Inchi:	InChI=1S/C6H10O3/c1-2-3-4-9-6(8)5-7/h5H,2-4H2,1H3
InchiKey:	NRYDRJHYTRBBEA-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CCCCOC(=O)C=O
Mol. weight [g/mol]:	130.14
CAS:	6295-06-3

Physical Properties

Property code	Value	Unit	Source
gf	-333.80	kJ/mol	Joback Method
hf	-497.55	kJ/mol	Joback Method
hfus	16.37	kJ/mol	Joback Method
hvap	44.83	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.529		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	461.63	K	Joback Method
tc	645.60	K	Joback Method
tf	271.54	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.79	J/molxK	461.63	Joback Method
cpg	225.84	J/molxK	492.29	Joback Method
cpg	234.55	J/molxK	522.95	Joback Method
cpg	242.94	J/molxK	553.61	Joback Method
cpg	251.00	J/molxK	584.27	Joback Method

cpg	258.72	J/mol×K	614.93	Joback Method
cpg	266.12	J/mol×K	645.60	Joback Method
dvisc	0.0030008	Paxs	271.54	Joback Method
dvisc	0.0017267	Paxs	303.22	Joback Method
dvisc	0.0011031	Paxs	334.90	Joback Method
dvisc	0.0007615	Paxs	366.58	Joback Method
dvisc	0.0005575	Paxs	398.27	Joback Method
dvisc	0.0004274	Paxs	429.95	Joback Method
dvisc	0.0003399	Paxs	461.63	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=C6295063&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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