Butyl glyoxalate

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

Physical Properties

Property code	Value	Unit	Source
af	0.5653		Cheméo Relay (1.0)
hf	-508.47	kJ/mol	Cheméo Relay (1.0)
hfus	16.37	kJ/mol	Joback Method
hvap	48.87	kJ/mol	Cheméo Relay (1.0)
ie	10.25	eV	Cheméo Relay (1.0)
log10ws	-1.06		Cheméo Relay (1.0)
logp	0.529		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	419.52	K	Cheméo Relay (1.0)
tc	627.91	K	Cheméo Relay (1.0)
tf	218.52	K	Cheméo Relay (1.0)
vc	0.395	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.79	J/mol×K	461.63	Joback Method
cpg	266.12	J/mol×K	645.60	Joback Method
cpg	258.72	J/mol×K	614.93	Joback Method
cpg	251.00	J/mol×K	584.27	Joback Method
cpg	242.94	J/mol×K	553.61	Joback Method

cpg	234.55	J/mol×K	522.95	Joback Method
cpg	225.84	J/mol×K	492.29	Joback Method
dvisc	0.0007615	Pa×s	366.59	Joback Method
dvisc	0.0003399	Pa×s	461.63	Joback Method
dvisc	0.0004274	Pa×s	429.95	Joback Method
dvisc	0.0005575	Pa×s	398.27	Joback Method
dvisc	0.0030008	Pa×s	271.54	Joback Method
dvisc	0.0011031	Pa×s	334.90	Joback Method
dvisc	0.0017267	Pa×s	303.22	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6295063&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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