

Ethyl 4-acetoxybutanoate

Inchi:	InChI=1S/C8H14O4/c1-3-11-8(10)5-4-6-12-7(2)9/h3-6H2,1-2H3
InchiKey:	KMPQIYXXLIFPKA-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	CCOC(=O)CCCOC(C)=O
Mol. weight [g/mol]:	174.19
CAS:	25560-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-451.36	kJ/mol	Joback Method
hf	-698.05	kJ/mol	Joback Method
hfus	22.05	kJ/mol	Joback Method
hvap	51.71	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.893		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1195.50		NIST Webbook
rinpol	1195.50		NIST Webbook
tb	535.02	K	Joback Method
tc	718.73	K	Joback Method
tf	324.24	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.22	J/mol×K	535.02	Joback Method
cpg	333.68	J/mol×K	565.64	Joback Method
cpg	344.72	J/mol×K	596.26	Joback Method
cpg	355.33	J/mol×K	626.88	Joback Method
cpg	365.50	J/mol×K	657.50	Joback Method
cpg	375.23	J/mol×K	688.12	Joback Method
cpg	384.50	J/mol×K	718.73	Joback Method

dvisc	0.0020386	Pa×s	324.24	Joback Method
dvisc	0.0011847	Pa×s	359.37	Joback Method
dvisc	0.0007583	Pa×s	394.50	Joback Method
dvisc	0.0005222	Pa×s	429.63	Joback Method
dvisc	0.0003804	Pa×s	464.76	Joback Method
dvisc	0.0002898	Pa×s	499.89	Joback Method
dvisc	0.0002287	Pa×s	535.02	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=C25560912&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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