

ethyl-«alpha»-ketobutyrate

Inchi:	InChI=1S/C6H10O3/c1-3-5(7)6(8)9-4-2/h3-4H2,1-2H3
InchiKey:	FJAKCEHATXBFJT-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CCOC(=O)C(=O)CC
Mol. weight [g/mol]:	130.14

Physical Properties

Property code	Value	Unit	Source
gf	-363.20	kJ/mol	Joback Method
hf	-524.55	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	44.85	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.529		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	1028.00		NIST Webbook
rinpol	1028.00		NIST Webbook
tb	466.84	K	Joback Method
tc	655.65	K	Joback Method
tf	279.47	K	Joback Method
vc	0.402	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.00	J/mol×K	466.84	Joback Method
cpg	258.27	J/mol×K	624.18	Joback Method
cpg	250.31	J/mol×K	592.71	Joback Method
cpg	242.00	J/mol×K	561.25	Joback Method
cpg	233.35	J/mol×K	529.78	Joback Method
cpg	224.34	J/mol×K	498.31	Joback Method
cpg	265.88	J/mol×K	655.65	Joback Method
dvisc	0.0003147	Paxs	466.84	Joback Method

dvisc	0.0003956	Paxs	435.61	Joback Method
dvisc	0.0005151	Paxs	404.38	Joback Method
dvisc	0.0007012	Paxs	373.16	Joback Method
dvisc	0.0010097	Paxs	341.93	Joback Method
dvisc	0.0015646	Paxs	310.70	Joback Method
dvisc	0.0026736	Paxs	279.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R494174&Units=SI

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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