

Ethyl pyrroacetate

Inchi: InChI=1S/C5H8O3/c1-3-8-5(7)4(2)6/h3H2,1-2H3
InchiKey: XXRCUYVCPSWGCC-UHFFFAOYSA-N
Formula: C5H8O3
SMILES: CCOC(=O)C(C)=O
Mol. weight [g/mol]: 116.12

Physical Properties

Property code	Value	Unit	Source
gf	-371.62	kJ/mol	Joback Method
hf	-503.91	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	0.138		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
ripol	1303.00		NIST Webbook
ripol	1303.00		NIST Webbook
tb	443.96	K	Joback Method
tc	634.74	K	Joback Method
tf	268.20	K	Joback Method
vc	0.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.41	J/molxK	443.96	Joback Method
cpg	184.43	J/molxK	475.76	Joback Method
cpg	192.17	J/molxK	507.55	Joback Method
cpg	199.65	J/molxK	539.35	Joback Method
cpg	206.83	J/molxK	571.15	Joback Method
cpg	213.74	J/molxK	602.95	Joback Method
cpg	220.34	J/molxK	634.74	Joback Method
dvisc	0.0025634	Paxs	268.20	Joback Method

dvisc	0.0015356	Paxs	297.49	Joback Method
dvisc	0.0010084	Paxs	326.79	Joback Method
dvisc	0.0007096	Paxs	356.08	Joback Method
dvisc	0.0005268	Paxs	385.37	Joback Method
dvisc	0.0004079	Paxs	414.67	Joback Method
dvisc	0.0003266	Paxs	443.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R608234&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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