Ethyl pyroracemate

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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0015356	Pa×s	297.49	Joback Method
dvisc	0.0010084	Pa×s	326.79	Joback Method
dvisc	0.0007096	Pa×s	356.08	Joback Method
dvisc	0.0005268	Pa×s	385.37	Joback Method
dvisc	0.0004079	Pa×s	414.67	Joback Method
dvisc	0.0003266	Pa×s	443.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R608234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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