Ethylcyclopropane carboxylate

Other names: Cyclopropanecarboxylic acid ethyl ester
Ethyl cyclopropylcarboxylate
Inchi: InChI=1S/C6H10O2/c1-2-8-6(7)5-3-4-5/h5H,2-4H2,1H3
InchiKey: LDDOSDVZPSGLFZ-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CCOC(=O)C1CC1
Mol. weight [g/mol]: 114.14

Physical Properties

Property code	Value	Unit	Source
af	0.4010		Cheméo Relay (1.0)
gf	-173.53	kJ/mol	Joback Method
hf	-379.48	kJ/mol	Cheméo Relay (1.0)
hfus	12.22	kJ/mol	Joback Method
hvap	43.39	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
log10ws	-1.37		Cheméo Relay (1.0)
logp	0.960		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	404.20	K	NIST Webbook
tc	610.94	K	Cheméo Relay (1.0)
tf	227.15	K	Cheméo Relay (1.0)
vc	0.348	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.77	J/mol×K	419.71	Joback Method
cpg	242.55	J/mol×K	612.36	Joback Method
cpg	233.99	J/mol×K	580.25	Joback Method
cpg	224.95	J/mol×K	548.14	Joback Method
cpg	215.43	J/mol×K	516.03	Joback Method
cpg	205.41	J/mol×K	483.93	Joback Method

cpg	194.86	J/mol×K	451.82	Joback Method
cpl	213.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0006880	Pa×s	333.59	Joback Method
dvisc	0.0004397	Pa×s	419.71	Joback Method
dvisc	0.0004994	Pa×s	391.00	Joback Method
dvisc	0.0005788	Pa×s	362.30	Joback Method
dvisc	0.0014699	Pa×s	247.48	Joback Method
dvisc	0.0008449	Pa×s	304.89	Joback Method
dvisc	0.0010828	Pa×s	276.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4606079&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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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