

Ethyl cyclobutanecarboxylate

Other names:	Cyclobutanecarboxylic acid, ethyl ester
Inchi:	InChI=1S/C7H12O2/c1-2-9-7(8)6-4-3-5-6/h6H,2-5H2,1H3
InchiKey:	SMVBADCAMQOTOV-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCOC(=O)C1CCC1
Mol. weight [g/mol]:	128.17
CAS:	14924-53-9

Physical Properties

Property code	Value	Unit	Source
chl	-4042.00	kJ/mol	NIST Webbook
gf	-177.21	kJ/mol	Joback Method
hf	-365.97	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	40.42	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.350		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	432.20	K	NIST Webbook
tc	645.24	K	Joback Method
tf	255.23	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.11	J/molxK	446.86	Joback Method
cpg	235.25	J/molxK	479.92	Joback Method
cpg	247.75	J/molxK	512.99	Joback Method
cpg	259.64	J/molxK	546.05	Joback Method
cpg	270.92	J/molxK	579.11	Joback Method
cpg	281.63	J/molxK	612.18	Joback Method
cpg	291.77	J/molxK	645.24	Joback Method

dvisc	0.0022676	Paxs	255.23	Joback Method
dvisc	0.0014442	Paxs	287.17	Joback Method
dvisc	0.0010067	Paxs	319.11	Joback Method
dvisc	0.0007494	Paxs	351.05	Joback Method
dvisc	0.0005860	Paxs	382.98	Joback Method
dvisc	0.0004759	Paxs	414.92	Joback Method
dvisc	0.0003982	Paxs	446.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14924539&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

chl:	Standard liquid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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