

Diethyl 1,1-cyclopropanedicarboxylate

Other names:	Diethyl cyclopropane-1,1-dicarboxylate 1,1-Cyclopropanedicarboxylic acid, diethyl ester
Inchi:	InChI=1S/C9H14O4/c1-3-12-7(10)9(5-6-9)8(11)13-4-2/h3-6H2,1-2H3
InchiKey:	KYYUCZOHNYSLFV-UHFFFAOYSA-N
Formula:	C9H14O4
SMILES:	CCOC(=O)C1(C(=O)OCC)CC1
Mol. weight [g/mol]:	186.21
CAS:	1559-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-387.68	kJ/mol	Joback Method
hf	-630.65	kJ/mol	Joback Method
hfus	16.48	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.893		Crippen Method
mvol	141.690	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	564.88	K	Joback Method
tc	766.58	K	Joback Method
tf	377.35	K	Joback Method
vc	0.542	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.24	J/mol×K	564.88	Joback Method
cpg	364.83	J/mol×K	598.50	Joback Method
cpg	376.73	J/mol×K	632.11	Joback Method
cpg	388.04	J/mol×K	665.73	Joback Method
cpg	398.82	J/mol×K	699.34	Joback Method
cpg	409.17	J/mol×K	732.96	Joback Method
cpg	419.17	J/mol×K	766.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1559020&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
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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