

Diethyl pyrocarbonate

Other names:	Diethyl oxydiformate Dicarbonic acid, diethyl ester Formic acid, oxydi-, diethyl ester Baycovin Depc Diethyl dicarbonate Diethylester kyseliny diuhlicite Diethyl ester of pyrocarbonic acid Diethyl pyrocarbonic acid Diethylpyrokarbonat DKD Ethyl pyrocarbonate Oxydiformic acid diethyl ester Piref Pyrocarbonate d'ethyle Pyrocarbonic acid, diethyl ester Pyrokohlensaeure diaethyl ester
Inchi:	InChI=1S/C6H10O5/c1-3-9-5(7)11-6(8)10-4-2/h3-4H2,1-2H3
InchiKey:	FFYPMLJYZAEMQB-UHFFFAOYSA-N
Formula:	C6H10O5
SMILES:	CCOC(=O)OC(=O)OCC
Mol. weight [g/mol]:	162.14
CAS:	1609-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-573.20	kJ/mol	Joback Method
hf	-788.99	kJ/mol	Joback Method
hfus	18.06	kJ/mol	Joback Method
hvap	49.67	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.316		Crippen Method
mcvol	116.150	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
tb	511.68	K	Joback Method
tc	698.40	K	Joback Method
tf	323.93	K	Joback Method

vc

0.438

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.98	J/mol×K	511.68	Joback Method
cpg	267.24	J/mol×K	542.80	Joback Method
cpg	276.25	J/mol×K	573.92	Joback Method
cpg	284.99	J/mol×K	605.04	Joback Method
cpg	293.42	J/mol×K	636.16	Joback Method
cpg	301.54	J/mol×K	667.28	Joback Method
cpg	309.31	J/mol×K	698.40	Joback Method
dvisc	0.0015736	Paxs	323.93	Joback Method
dvisc	0.0009820	Paxs	355.22	Joback Method
dvisc	0.0006614	Paxs	386.51	Joback Method
dvisc	0.0004727	Paxs	417.81	Joback Method
dvisc	0.0003540	Paxs	449.10	Joback Method
dvisc	0.0002752	Paxs	480.39	Joback Method
dvisc	0.0002207	Paxs	511.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.70	K	2.40	NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1609478&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

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
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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