

Ethyl neopentyl carbonate

Inchi:

InChI=1S/C8H16O3/c1-5-10-7(9)11-6-8(2,3)4/h5-6H2,1-4H3

InchiKey:

DXGMUSVPWXDDID-UHFFFAOYSA-N

Formula:

C8H16O3

SMILES:

CCOC(=O)OCC(C)(C)C

Mol. weight [g/mol]:

160.21

Physical Properties

Property code	Value	Unit	Source
gf	-319.60	kJ/mol	Joback Method
hf	-594.22	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	43.67	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	2.206		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	972.00		NIST Webbook
tb	477.92	K	Joback Method
tc	663.13	K	Joback Method
tf	276.73	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.74	J/mol×K	477.92	Joback Method
cpg	366.89	J/mol×K	632.26	Joback Method
cpg	355.92	J/mol×K	601.39	Joback Method
cpg	344.43	J/mol×K	570.52	Joback Method
cpg	332.41	J/mol×K	539.66	Joback Method
cpg	319.85	J/mol×K	508.79	Joback Method
cpg	377.34	J/mol×K	663.13	Joback Method
dvisc	0.0002119	Pa×s	477.92	Joback Method
dvisc	0.0002813	Pa×s	444.39	Joback Method

dvisc	0.0003911	Pa×s	410.86	Joback Method
dvisc	0.0005766	Pa×s	377.32	Joback Method
dvisc	0.0009170	Pa×s	343.79	Joback Method
dvisc	0.0016120	Pa×s	310.26	Joback Method
dvisc	0.0032491	Pa×s	276.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373765&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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