

Carbonic acid, heptyl methyl ester

Other names:	Methyl heptyl carbonate
Inchi:	InChI=1S/C9H18O3/c1-3-4-5-6-7-8-12-9(10)11-2/h3-8H2,1-2H3
InchiKey:	IBTAFYOTPNVGLR-UHFFFAOYSA-N
Formula:	C9H18O3
SMILES:	CCCCCCCOC(=O)OC
Mol. weight [g/mol]:	174.24

Physical Properties

Property code	Value	Unit	Source
gf	-314.02	kJ/mol	Joback Method
hf	-606.11	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	47.19	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.740		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1166.60		NIST Webbook
tb	504.03	K	Joback Method
tc	677.20	K	Joback Method
tf	285.58	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.03	J/molxK	504.03	Joback Method
cpg	361.09	J/molxK	532.89	Joback Method
cpg	373.72	J/molxK	561.75	Joback Method
cpg	385.91	J/molxK	590.62	Joback Method
cpg	397.66	J/molxK	619.48	Joback Method
cpg	408.97	J/molxK	648.34	Joback Method
cpg	419.82	J/molxK	677.20	Joback Method
dvisc	0.0024200	Paxs	285.58	Joback Method

dvisc	0.0012601	Paxs	321.99	Joback Method
dvisc	0.0007491	Paxs	358.40	Joback Method
dvisc	0.0004902	Paxs	394.81	Joback Method
dvisc	0.0003446	Paxs	431.21	Joback Method
dvisc	0.0002559	Paxs	467.62	Joback Method
dvisc	0.0001984	Paxs	504.03	Joback Method

Sources

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=U314619&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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