

2,4-Dimethylpentan-3-yl ethyl carbonate

Inchi:	InChI=1S/C10H20O3/c1-6-12-10(11)13-9(7(2)3)8(4)5/h7-9H,6H2,1-5H3
InchiKey:	GTRBOBAVUJEMQK-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	CCOC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	188.26

Physical Properties

Property code	Value	Unit	Source
gf	-312.92	kJ/mol	Joback Method
hf	-642.59	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	48.26	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.840		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinsol	1115.00		NIST Webbook
tb	525.59	K	Joback Method
tc	707.71	K	Joback Method
tf	251.85	K	Joback Method
vc	0.620	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.97	J/molxK	525.59	Joback Method
cpg	409.95	J/molxK	555.94	Joback Method
cpg	424.37	J/molxK	586.30	Joback Method
cpg	438.21	J/molxK	616.65	Joback Method
cpg	451.48	J/molxK	647.01	Joback Method
cpg	464.17	J/molxK	677.36	Joback Method
cpg	476.28	J/molxK	707.71	Joback Method
dvisc	0.0070821	Paxs	251.85	Joback Method
dvisc	0.0022874	Paxs	297.47	Joback Method

dvisc	0.0009978	Paxs	343.10	Joback Method
dvisc	0.0005288	Paxs	388.72	Joback Method
dvisc	0.0003203	Paxs	434.34	Joback Method
dvisc	0.0002134	Paxs	479.97	Joback Method
dvisc	0.0001525	Paxs	525.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373796&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_cvol:	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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