

Prop-2-ynyl propyl carbonate

Inchi:	InChI=1S/C7H10O3/c1-3-5-9-7(8)10-6-4-2/h1H,4-6H2,2H3
InchiKey:	LIONVJNHPDUBMD-UHFFFAOYSA-N
Formula:	C7H10O3
SMILES:	C#CCOC(=O)OCCC
Mol. weight [g/mol]:	142.15

Physical Properties

Property code	Value	Unit	Source
gf	-107.79	kJ/mol	Joback Method
hf	-272.93	kJ/mol	Joback Method
hfus	20.84	kJ/mol	Joback Method
hvap	42.60	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.183		Crippen Method
mcvol	114.200	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
tb	448.39	K	Joback Method
tc	636.63	K	Joback Method
tf	310.01	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.12	J/mol×K	448.39	Joback Method
cpg	241.47	J/mol×K	479.76	Joback Method
cpg	250.53	J/mol×K	511.14	Joback Method
cpg	259.27	J/mol×K	542.51	Joback Method
cpg	267.71	J/mol×K	573.89	Joback Method
cpg	275.83	J/mol×K	605.26	Joback Method
cpg	283.63	J/mol×K	636.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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