

Carbonic acid, propargyl phenyl ester

Inchi: InChI=1S/C10H8O3/c1-2-8-12-10(11)13-9-6-4-3-5-7-9/h1,3-7H,8H2
InchiKey: QDKDRURRUQJPAD-UHFFFAOYSA-N
Formula: C10H8O3
SMILES: C#CCOC(=O)Oc1ccccc1
Mol. weight [g/mol]: 176.17

Physical Properties

Property code	Value	Unit	Source
gf	29.88	kJ/mol	Joback Method
hf	-98.32	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Joback Method
hvap	51.55	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.835		Crippen Method
mcvol	132.710	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
tb	543.71	K	Joback Method
tc	769.49	K	Joback Method
tf	370.24	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.39	J/mol×K	543.71	Joback Method
cpg	299.16	J/mol×K	581.34	Joback Method
cpg	310.24	J/mol×K	618.97	Joback Method
cpg	320.62	J/mol×K	656.60	Joback Method
cpg	330.31	J/mol×K	694.23	Joback Method
cpg	339.33	J/mol×K	731.86	Joback Method
cpg	347.69	J/mol×K	769.49	Joback Method

Sources

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=U357908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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