Carbonic acid, propargyl 2-ethylhexyl ester

Inchi: InChI=1S/C12H20O3/c1-4-7-8-11(6-3)10-15-12(13)14-9-5-2/h2,11H,4,6-10H2,1,3H3
InchiKey: QOJFGFLSHWRPKO-UHFFFAOYSA-N
Formula: C12H20O3
SMILES: C#CCOC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-68.13	kJ/mol	Joback Method
hf	-381.41	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	53.34	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.989		Crippen Method
mcvol	184.650	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1418.00		NIST Webbook
tb	562.35	K	Joback Method
tc	744.63	K	Joback Method
tf	351.36	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.33	J/mol×K	562.35	Joback Method
cpg	467.06	J/mol×K	592.73	Joback Method
cpg	481.17	J/mol×K	623.11	Joback Method
cpg	494.68	J/mol×K	653.49	Joback Method
cpg	507.58	J/mol×K	683.87	Joback Method
cpg	519.88	J/mol×K	714.25	Joback Method
cpg	531.59	J/mol×K	744.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357909&Units=SI
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

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