

Carbonic acid, allyl 2-ethylhexyl ester

Inchi:	InChI=1S/C12H22O3/c1-4-7-8-11(6-3)10-15-12(13)14-9-5-2/h5,11H,2,4,6-10H2,1,3H3
InchiKey:	RAEACIVHTRRGpz-UHFFFAOYSA-N
Formula:	C12H22O3
SMILES:	C=CCOC(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	214.30

Physical Properties

Property code	Value	Unit	Source
gf	-203.36	kJ/mol	Joback Method
hf	-547.88	kJ/mol	Joback Method
hfus	26.01	kJ/mol	Joback Method
hvap	52.81	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.542		Crippen Method
mvol	188.950	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	1393.00		NIST Webbook
tb	568.91	K	Joback Method
tc	744.16	K	Joback Method
tf	302.63	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.92	J/molxK	568.91	Joback Method
cpg	542.08	J/molxK	714.95	Joback Method
cpg	529.26	J/molxK	685.74	Joback Method
cpg	515.84	J/molxK	656.53	Joback Method
cpg	501.81	J/molxK	627.33	Joback Method
cpg	487.17	J/molxK	598.12	Joback Method
cpg	554.30	J/molxK	744.16	Joback Method
dvisc	0.0001453	Paxs	568.91	Joback Method
dvisc	0.0001928	Paxs	524.53	Joback Method

dvisc	0.0002696	Paxs	480.15	Joback Method
dvisc	0.0004037	Paxs	435.77	Joback Method
dvisc	0.0006625	Paxs	391.39	Joback Method
dvisc	0.0012340	Paxs	347.01	Joback Method
dvisc	0.0027584	Paxs	302.63	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=U357806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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