

Carbonic acid, 2-methoxyethyl 3,5-dimethylphenyl ester

Inchi:	InChI=1S/C12H16O4/c1-9-6-10(2)8-11(7-9)16-12(13)15-5-4-14-3/h6-8H,4-5H2,1-3H3
InchiKey:	MFDNRMIPDYDWAU-UHFFFAOYSA-N
Formula:	C12H16O4
SMILES:	COCCOC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	224.25

Physical Properties

Property code	Value	Unit	Source
gf	-300.61	kJ/mol	Joback Method
hf	-586.66	kJ/mol	Joback Method
hfus	25.26	kJ/mol	Joback Method
hvap	59.88	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.465		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1673.00		NIST Webbook
tb	631.73	K	Joback Method
tc	835.57	K	Joback Method
tf	393.08	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.38	J/molxK	631.73	Joback Method
cpg	458.60	J/molxK	665.70	Joback Method
cpg	472.11	J/molxK	699.68	Joback Method
cpg	484.90	J/molxK	733.65	Joback Method
cpg	496.95	J/molxK	767.63	Joback Method
cpg	508.24	J/molxK	801.60	Joback Method
cpg	518.77	J/molxK	835.57	Joback Method
dvisc	0.0007650	Paxs	393.08	Joback Method
dvisc	0.0004811	Paxs	432.86	Joback Method

dvisc	0.0003272	Paxs	472.63	Joback Method
dvisc	0.0002362	Paxs	512.40	Joback Method
dvisc	0.0001787	Paxs	552.18	Joback Method
dvisc	0.0001404	Paxs	591.96	Joback Method
dvisc	0.0001137	Paxs	631.73	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=U357873&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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