Carbamic acid, phenyl-, ethyl ester

Other names:	Carbanilic acid, ethyl ester
	Ethyl carbanilate
	Ethyl phenylcarbamate
	Ethyl N-phenylcarbamate
	Ethyl N-phenylurethan
	Ethyl N-phenylurethane
	Euphorin
	EPC (The plant regulator)
	Keimstop
	N-(Ethoxycarbonyl)aniline
	N-Phenylurethane
	Phenylurethan
	Phenylurethane
	Phenylethyl carbamate
	Urethane, phenyl-
	EPC
	Ethylester kyseliny karbanilove
	Urethan, phenyl-
	Ethyl ester of phenylcarbamic acid
	Ethyl N-phenylcarbanilate
	N-Phenyl ethylcarbamate
	Phenylcarbamic acid ethyl ester
	Carbamic acid, N-phenyl-, ethyl ester
	Ethanol, carbanilate
	NSC 3245
Inchi:	InChI=1S/C9H11NO2/c1-2-12-9(11)10-8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H,10,11)
InchiKey:	LBKPGNUOUPTQKA-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	CCOC(=O)Nc1ccccc1
Mol. weight [g/mol]:	165.19
CAS:	101-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-7.22	kJ/mol	Joback Method
hf	-183.89	kJ/mol	Joback Method

hfus	20.99	kJ/mol	Joback Method
hvap	53.50	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.255		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1401.00		NIST Webbook
ripol	2031.00		NIST Webbook
ripol	2031.00		NIST Webbook
tb	558.46	K	Joback Method
tc	774.81	K	Joback Method
tf	326.00 ± 1.00	K	NIST Webbook
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.48	J/mol×K	630.58	Joback Method
cpg	367.10	J/mol×K	774.81	Joback Method
cpg	358.00	J/mol×K	738.75	Joback Method
cpg	348.21	J/mol×K	702.69	Joback Method
cpg	337.71	J/mol×K	666.64	Joback Method
cpg	301.77	J/mol×K	558.46	Joback Method
cpg	314.51	J/mol×K	594.52	Joback Method
cps	227.20	J/mol×K	298.00	NIST Webbook
hfust	16.27	kJ/mol	326.00	NIST Webbook
hfust	16.27	kJ/mol	326.00	NIST Webbook
hfust	16.27	kJ/mol	326.00	NIST Webbook
hvapt	84.20	kJ/mol	445.00	NIST Webbook
sfust	49.90	J/mol×K	326.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101995&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

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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