

Ethyl allophanate

Other names:	Allophanic acid ethyl ester Carbamic acid, (aminocarbonyl)-, ethyl ester ethyl (aminocarbonyl)carbamate
Inchi:	InChI=1S/C4H8N2O3/c1-2-9-4(8)6-3(5)7/h2H2,1H3,(H3,5,6,7,8)
InchiKey:	PIHPSKJRLDSJPX-UHFFFAOYSA-N
Formula:	C4H8N2O3
SMILES:	CCOC(=O)NC(N)=O
Mol. weight [g/mol]:	132.12
CAS:	626-36-8

Physical Properties

Property code	Value	Unit	Source
gf	-224.20	kJ/mol	Joback Method
hf	-396.01	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	57.48	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	-0.189		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
tb	543.78	K	Joback Method
tc	749.98	K	Joback Method
tf	392.85	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.70	J/molxK	543.78	Joback Method
cpg	228.76	J/molxK	578.15	Joback Method
cpg	236.43	J/molxK	612.51	Joback Method
cpg	243.71	J/molxK	646.88	Joback Method
cpg	250.60	J/molxK	681.25	Joback Method
cpg	257.09	J/molxK	715.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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