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

Physical Properties

Property code	Value	Unit	Source
af	0.6713		Cheméo Relay (1.0)
gf	-224.20	kJ/mol	Joback Method
hf	-668.61	kJ/mol	Cheméo Relay (1.0)
hfus	20.80	kJ/mol	Joback Method
hvap	72.78	kJ/mol	Cheméo Relay (1.0)
ie	9.73	eV	Cheméo Relay (1.0)
log10ws	-1.28		Cheméo Relay (1.0)
logp	-0.189		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
tb	494.35	K	Cheméo Relay (1.0)
tc	692.49	K	Cheméo Relay (1.0)
tf	382.75	K	Cheméo Relay (1.0)
vc	0.358	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	257.09	J/mol×K	715.61	Joback Method
cpg	263.18	J/mol×K	749.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626368&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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