Carbamic acid, N-phenyl-, heptyl ester

Other names: Carbamic acid, N-phenyl-, heptyl ester
Inchi: InChI=1S/C14H21NO2/c1-2-3-4-5-9-12-17-14(16)15-13-10-7-6-8-11-13/h6-8,10-11H,2-5
InchiKey: OJXUXLGVKNOXFM-UHFFFAOYSA-N
Formula: C14H21NO2
SMILES: CCCCCCCOC(=O)Nc1ccccc1
Mol. weight [g/mol]: 235.33

Physical Properties

Property code	Value	Unit	Source
af	0.7849		Cheméo Relay (1.0)
hf	-409.90	kJ/mol	Cheméo Relay (1.0)
hfus	33.94	kJ/mol	Joback Method
hvap	88.18	kJ/mol	Cheméo Relay (1.0)
ie	8.31	eV	Cheméo Relay (1.0)
log10ws	-4.68		Cheméo Relay (1.0)
logp	4.205		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
tb	590.43	K	Cheméo Relay (1.0)
tc	824.28	K	Cheméo Relay (1.0)
tf	316.23	K	Cheméo Relay (1.0)
vc	0.746	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.62	J/mol×K	672.86	Joback Method
cpg	565.43	J/mol×K	706.28	Joback Method
cpg	580.31	J/mol×K	739.70	Joback Method
cpg	594.29	J/mol×K	773.12	Joback Method
cpg	607.39	J/mol×K	806.54	Joback Method
cpg	619.65	J/mol×K	839.96	Joback Method
cpg	631.08	J/mol×K	873.38	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109562392&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):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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