

Carbamic acid, N-(4-nitrophenyl)-, heptyl ester

Other names:	Carbamic acid, N-(4-nitrophenyl)-, heptyl ester
Inchi:	InChI=1S/C14H20N2O4/c1-2-3-4-5-6-11-20-14(17)15-12-7-9-13(10-8-12)16(18)19/h7-10
InchiKey:	PJOBNIUGOZOAFD-UHFFFAOYSA-N
Formula:	C14H20N2O4
SMILES:	CCCCCCCCOC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	280.32

Physical Properties

Property code	Value	Unit	Source
hf	-426.83	kJ/mol	Cheméo Relay (1.0)
hfus	44.91	kJ/mol	Joback Method
hvap	106.66	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-5.06		Cheméo Relay (1.0)
logp	4.114		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
tb	615.98	K	Cheméo Relay (1.0)
tf	360.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.10	J/mol×K	829.68	Joback Method
cpg	671.30	J/mol×K	866.57	Joback Method
cpg	683.47	J/mol×K	903.47	Joback Method
cpg	694.64	J/mol×K	940.36	Joback Method
cpg	704.85	J/mol×K	977.26	Joback Method
cpg	714.13	J/mol×K	1014.15	Joback Method
cpg	722.52	J/mol×K	1051.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92374997&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

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
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/119-773-2/Carbamic-acid-N-4-nitrophenyl-heptyl-ester.pdf>

Generated by Cheméo on 2026-07-21 14:30:46.592184416 +0000 UTC m=+155342.434069796.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.