

Placidyl carbamate

Inchi:	InChI=1S/C8H10CINO2/c1-3-8(4-2,5-6-9)12-7(10)11/h1,5-6H,4H2,2H3,(H2,10,11)/b6-5+
InchiKey:	FCCBKWLMYXVTGQ-AATRIKPKSA-N
Formula:	C8H10CINO2
SMILES:	C#CC(C=CCI)(CC)OC(N)=O
Mol. weight [g/mol]:	187.62
CAS:	74283-25-3

Physical Properties

Property code	Value	Unit	Source
gf	143.21	kJ/mol	Joback Method
hf	-34.83	kJ/mol	Joback Method
hfus	24.42	kJ/mol	Joback Method
hvap	56.10	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	1.616		Crippen Method
mcvol	140.340	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	559.74	K	Joback Method
tc	785.41	K	Joback Method
tf	409.57	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.11	J/molxK	559.74	Joback Method
cpg	321.68	J/molxK	597.35	Joback Method
cpg	331.47	J/molxK	634.96	Joback Method
cpg	340.52	J/molxK	672.58	Joback Method
cpg	348.90	J/molxK	710.19	Joback Method
cpg	356.66	J/molxK	747.80	Joback Method
cpg	363.86	J/molxK	785.41	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74283253&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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