

N-Propylamphetamine, N-propyloxycarbonyl-

Other names:	N-Propylamphetamine, N-propoxycarbonyl
Inchi:	InChI=1S/C16H25NO2/c1-4-11-17(16(18)19-12-5-2)14(3)13-15-9-7-6-8-10-15/h6-10,14H
InchiKey:	JGNZCOXDHFFGQV-UHFFFAOYSA-N
Formula:	C16H25NO2
SMILES:	CCCOC(=O)N(CCC)C(C)Cc1ccccc1
Mol. weight [g/mol]:	263.38

Physical Properties

Property code	Value	Unit	Source
gf	70.67	kJ/mol	Joback Method
hf	-319.59	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.876		Crippen Method
mvol	229.960	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
tb	680.45	K	Joback Method
tc	877.00	K	Joback Method
tf	386.13	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.42	J/molxK	680.45	Joback Method
cpg	658.06	J/molxK	713.21	Joback Method
cpg	674.67	J/molxK	745.97	Joback Method
cpg	690.27	J/molxK	778.73	Joback Method
cpg	704.92	J/molxK	811.49	Joback Method
cpg	718.63	J/molxK	844.24	Joback Method
cpg	731.46	J/molxK	877.00	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U314782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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