

Phenprobamate

Other names:	Benzenepropanol, carbamate «gamma»-Phenylpropyl carbamate Actiphan Actozine Ansepron Carbamic acid, 3-phenylpropyl ester Eirenal Extacol Fenprobamato Gamaquil HG 532 MH 532 Nelaxan Palmita Phenoprobamate Proformiphen Qumamquil Spantol Tranquil 1-Carbamoyloxy-3-phenylpropane 1-Propanol, 3-phenyl-, carbamate 3-Phenyl-1-propanol carbamate 3-Phenylpropyl carbamate Quamaquil NSC 44682 NSC 50538
Inchi:	InChI=1S/C10H13NO2/c11-10(12)13-8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7-8H2,(H2,11,12)
InchiKey:	CAMYKONBWHRPDD-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	NC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	179.22
CAS:	673-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-21.74	kJ/mol	Joback Method

hf	-224.21		kJ/mol	Joback Method
h _{fus}	23.68		kJ/mol	Joback Method
h _{vap}	59.93		kJ/mol	Joback Method
log ₁₀ w _s	-2.39			Crippen Method
log _p	1.715			Crippen Method
m _{cvol}	145.420		ml/mol	McGowan Method
pc	3287.81		kPa	Joback Method
tb	603.70		K	Joback Method
tc	824.85		K	Joback Method
tf	376.50 ± 0.50		K	NIST Webbook
vc	0.540		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
c _{pg}	357.93	J/mol×K	603.70	Joback Method
c _{pg}	371.21	J/mol×K	640.56	Joback Method
c _{pg}	383.65	J/mol×K	677.42	Joback Method
c _{pg}	395.27	J/mol×K	714.27	Joback Method
c _{pg}	406.09	J/mol×K	751.13	Joback Method
c _{pg}	416.14	J/mol×K	787.99	Joback Method
c _{pg}	425.45	J/mol×K	824.85	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=C673314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

c_{pg}:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	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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