

Emylcamate

Other names:	3-Pentanol, 3-methyl-, carbamate tert-Hexanol carbamate Diethyl methyl carbinol urethan Emylcamat KABI-925 Methyl Diethyl carbinol urethan MK-250 Nuncital Statran Striatan Striatran 1-Ethyl-1-Methylpropyl carbamate 3-Methyl-3-pentanol carbamate 91 JD Carbamic acid, 1-ethyl-1-methylpropyl ester Emilcamato JD-91 Kabi-295 Psicoplegil Restetal Stratran Carbamic acid, tert-hexyl ester tert-Hexyl carbamate terc.Hexylester kyseliny karbaminove Stratan NSC 169882
Inchi:	InChI=1S/C7H15NO2/c1-4-7(3,5-2)10-6(8)9/h4-5H2,1-3H3,(H2,8,9)
InchiKey:	SLWGJZPKHAXZQL-UHFFFAOYSA-N
Formula:	C7H15NO2
SMILES:	CCC(C)(CC)OC(N)=O
Mol. weight [g/mol]:	145.20
CAS:	78-28-4

Physical Properties

Property code	Value	Unit	Source
gf	-156.57	kJ/mol	Joback Method

hf	-407.57		kJ/mol	Joback Method
hfus	14.46		kJ/mol	Joback Method
hvap	49.68		kJ/mol	Joback Method
log10ws	-2.14			Crippen Method
logp	1.660			Crippen Method
mcvol	126.910		ml/mol	McGowan Method
pc	3199.16		kPa	Joback Method
rinpol	1105.00			NIST Webbook
rinpol	1105.00			NIST Webbook
tb	505.15		K	Joback Method
tc	704.95		K	Joback Method
tf	326.49		K	Joback Method
vc	0.469		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.86	J/mol×K	505.15	Joback Method
cpg	309.45	J/mol×K	538.45	Joback Method
cpg	321.38	J/mol×K	571.75	Joback Method
cpg	332.68	J/mol×K	605.05	Joback Method
cpg	343.37	J/mol×K	638.35	Joback Method
cpg	353.46	J/mol×K	671.65	Joback Method
cpg	362.98	J/mol×K	704.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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