

Tolycaine

Other names:	Benzoic acid, 2-[[[(diethylamino)acetyl]amino]-3-methyl-, methyl ester Methyl 2-[2-(diethylamino)acetamido]-m-toluate
Inchi:	InChI=1S/C15H22N2O3/c1-5-17(6-2)10-13(18)16-14-11(3)8-7-9-12(14)15(19)20-4/h7-9H
InchiKey:	UDKICLZCJWQTLS-UHFFFAOYSA-N
Formula:	C15H22N2O3
SMILES:	CCN(CC)CC(=O)Nc1c(C)cccc1C(=O)OC
Mol. weight [g/mol]:	278.35
CAS:	3686-58-6

Physical Properties

Property code	Value	Unit	Source
gf	5.90	kJ/mol	Joback Method
hf	-375.72	kJ/mol	Joback Method
hfus	40.38	kJ/mol	Joback Method
hvap	76.97	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.062		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
tb	772.01	K	Joback Method
tc	976.81	K	Joback Method
tf	517.49	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.89	J/mol×K	772.01	Joback Method
cpg	675.37	J/mol×K	806.14	Joback Method
cpg	688.88	J/mol×K	840.28	Joback Method
cpg	701.45	J/mol×K	874.41	Joback Method
cpg	713.11	J/mol×K	908.55	Joback Method
cpg	723.88	J/mol×K	942.68	Joback Method
cpg	733.79	J/mol×K	976.81	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=C3686586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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