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

Physical Properties

Property code	Value	Unit	Source
hf	-510.51	kJ/mol	Cheméo Relay (1.0)
hfus	40.38	kJ/mol	Joback Method
ie	7.51	eV	Cheméo Relay (1.0)
log10ws	-2.33		Cheméo Relay (1.0)
logp	2.062		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
tb	604.62	K	Cheméo Relay (1.0)
tf	368.89	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3686586&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point