Acetylprocaine

Other names: 2-diethylaminoethyl 4-acetamidobenzoate
Inchi: InChI=1S/C15H22N2O3/c1-4-17(5-2)10-11-20-15(19)13-6-8-14(9-7-13)16-12(3)18/h6-9H
InchiKey: YMABTXMPJQRLCQ-UHFFFAOYSA-N
Formula: C15H22N2O3
SMILES: CCN(CC)CCOC(=O)c1ccc(NC(C)=O)cc1
Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
gf	15.53	kJ/mol	Joback Method
hf	-364.25	kJ/mol	Joback Method
hfus	40.76	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-1.65		Aqueous Solubility Prediction Method
logp	2.144		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	767.03	K	Joback Method
tc	971.03	K	Joback Method
tf	504.97	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.81	J/mol×K	767.03	Joback Method
cpg	676.39	J/mol×K	801.03	Joback Method
cpg	689.99	J/mol×K	835.03	Joback Method
cpg	702.64	J/mol×K	869.03	Joback Method

cpg	714.37	J/mol×K	903.03	Joback Method
cpg	725.21	J/mol×K	937.03	Joback Method
cpg	735.21	J/mol×K	971.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U379134&Units=SI

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