2-hydroxy-2',6'-diethyl-N-acetanilide

Inchi: InChI=1S/C12H17NO2/c1-3-9-6-5-7-10(4-2)12(9)13-11(15)8-14/h5-7,14H,3-4,8H2,1-2H3
InchiKey: JQQZSHMUVAYCDW-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CCc1cccc(CC)c1NC(=O)CO
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	-33.04	kJ/mol	Joback Method
hf	-288.76	kJ/mol	Joback Method
hfus	30.89	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	1.742		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	306.40		NIST Webbook
rinpol	1889.00		NIST Webbook
rinpol	306.40		NIST Webbook
rinpol	1889.00		NIST Webbook
tb	706.82	K	Joback Method
tc	904.70	K	Joback Method
tf	439.87	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.72	J/mol×K	706.82	Joback Method
cpg	485.79	J/mol×K	739.80	Joback Method
cpg	497.15	J/mol×K	772.78	Joback Method
cpg	507.84	J/mol×K	805.76	Joback Method
cpg	517.87	J/mol×K	838.74	Joback Method

cpg	527.28	J/mol×K	871.72	Joback Method
cpg	536.09	J/mol×K	904.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R408514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume