4-Diethylamino-2-methyl acetanilide

Inchi: InChI=1S/C13H20N2O/c1-5-15(6-2)12-7-8-13(10(3)9-12)14-11(4)16/h7-9H,5-6H2,1-4H3
InchiKey: ORCJVXMOXNZNAY-UHFFFAOYSA-N
Formula: C13H20N2O
SMILES: CCN(CC)c1ccc(NC(C)=O)c(C)c1
Mol. weight [g/mol]: 220.31
CAS: 5417-52-7

Physical Properties

Property code	Value	Unit	Source
gf	222.98	kJ/mol	Joback Method
hf	-89.64	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	63.36	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.800		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
tb	649.96	K	Joback Method
tc	854.18	K	Joback Method
tf	422.79	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.64	J/mol×K	649.96	Joback Method
cpg	523.28	J/mol×K	684.00	Joback Method
cpg	538.00	J/mol×K	718.03	Joback Method
cpg	551.83	J/mol×K	752.07	Joback Method
cpg	564.81	J/mol×K	786.10	Joback Method
cpg	576.99	J/mol×K	820.14	Joback Method
cpg	588.38	J/mol×K	854.18	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=C5417527&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