N,N-dimethylphenylglycine

Inchi: InChI=1S/C10H13NO2/c1-11(2)9(10(12)13)8-6-4-3-5-7-8/h3-7,9H,1-2H3,(H,12,13)
InchiKey: MLOBRLOZPSSKKO-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CN(C)C(C(=O)O)c1ccccc1
Mol. weight [g/mol]: 179.22

Physical Properties

Property code	Value	Unit	Source
gf	-11.67	kJ/mol	Joback Method
hf	-215.76	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	65.21	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.374		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
ripol	2037.00		NIST Webbook
ripol	2037.00		NIST Webbook
tb	612.93	K	Joback Method
tc	814.53	K	Joback Method
tf	357.10	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.00	J/mol×K	612.93	Joback Method
cpg	376.06	J/mol×K	646.53	Joback Method
cpg	387.35	J/mol×K	680.13	Joback Method
cpg	397.88	J/mol×K	713.73	Joback Method
cpg	407.72	J/mol×K	747.33	Joback Method
cpg	416.88	J/mol×K	780.93	Joback Method
cpg	425.41	J/mol×K	814.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R398046&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume