4-Dimethylaminonaphthalene-1-carboxylic acid

Inchi: InChI=1S/C13H13NO2/c1-14(2)12-8-7-11(13(15)16)9-5-3-4-6-10(9)12/h3-8H,1-2H3,(H,1

InchiKey: LZQKNRRVTOJUHQ-UHFFFAOYSA-N

Formula: C13H13NO2

SMILES: CN(C)c1ccc(C(=O)O)c2ccccc12

Mol. weight [g/mol]: 215.25

CAS: 78062-03-0

Physical Properties

Property code	Value	Unit	Source
gf	103.42	kJ/mol	Joback Method
hf	-104.27	kJ/mol	Joback Method
hfus	28.42	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.604		Crippen Method
mcvol	168.230	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	710.95	K	Joback Method
tc	924.65	K	Joback Method
tf	463.65	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.39	J/mol×K	710.95	Joback Method
cpg	457.81	J/mol×K	746.57	Joback Method
cpg	468.45	J/mol×K	782.18	Joback Method
cpg	478.37	J/mol×K	817.80	Joback Method
cpg	487.64	J/mol×K	853.41	Joback Method
cpg	496.33	J/mol×K	889.03	Joback Method
cpg	504.49	J/mol×K	924.65	Joback Method

Sources

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=C78062030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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