4-(Diethylamino)benzoic acid

Other names:	4-N,N-Diethylaminobenzoic acid
	p-Diethylaminobenzoic acid
	Benzoic acid, 4-(diethylamino)-
Inchi:	InChI=1S/C11H15NO2/c1-3-12(4-2)10-7-5-9(6-8-10)11(13)14/h5-8H,3-4H2,1-2H3,(H,13,
InchiKey:	LNYTUARMNSFFBE-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CCN(CC)c1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	193.24
CAS:	5429-28-7

Physical Properties

Property code	Value	Unit	Source
gf	-10.44	kJ/mol	Joback Method
hf	-242.59	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	68.49	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.231		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	641.23	K	Joback Method
tc	837.46	K	Joback Method
tf	395.89	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.48	J/mol×K	641.23	Joback Method
cpg	423.71	J/mol×K	673.93	Joback Method
cpg	435.21	J/mol×K	706.64	Joback Method
cpg	446.00	J/mol×K	739.34	Joback Method
cpg	456.13	J/mol×K	772.05	Joback Method
cpg	465.63	J/mol×K	804.75	Joback Method

cpg	474.53	J/mol×K	837.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5429287&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume