Methyl 3,4-diaminobenzoate

Inchi: InChI=1S/C8H10N2O2/c1-12-8(11)5-2-3-6(9)7(10)4-5/h2-4H,9-10H2,1H3
InchiKey: IOPLHGOSNCJOOO-UHFFFAOYSA-N
Formula: C8H10N2O2
SMILES: COC(=O)c1ccc(N)c(N)c1
Mol. weight [g/mol]: 166.18
CAS: 36692-49-6

Physical Properties

Property code	Value	Unit	Source
gf	8.61	kJ/mol	Joback Method
hf	-172.08	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	67.44	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	0.638		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	640.43	K	Joback Method
tc	879.35	K	Joback Method
tf	470.06	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.21	J/mol×K	640.43	Joback Method
cpg	326.00	J/mol×K	680.25	Joback Method
cpg	336.07	J/mol×K	720.07	Joback Method
cpg	345.42	J/mol×K	759.89	Joback Method
cpg	354.05	J/mol×K	799.71	Joback Method
cpg	361.98	J/mol×K	839.53	Joback Method
cpg	369.21	J/mol×K	879.35	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=C36692496&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