2-Anisamide

Other names:	2-methoxybenzamide
	Benzamide, 2-methoxy-
	Benzamide, o-methoxy-
	H.P. 208
	o-anisamide
	o-methoxybenzamide
Inchi:	InChI=1S/C8H9NO2/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3,(H2,9,10)
InchiKey:	MNWSGMTUGXNYHJ-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	COc1ccccc1C(N)=O
Mol. weight [g/mol]:	151.17

Physical Properties

Property code	Value	Unit	Source
hf	-284.78	kJ/mol	Cheméo Relay (1.0)
hfus	27.21	kJ/mol	The thermodynamic stability of the three isomers of methoxybenzamide: An experimental and computational study
hvap	70.14	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-1.97		Cheméo Relay (1.0)
logp	0.794		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
tb	558.99	K	Cheméo Relay (1.0)
tc	773.47	K	Cheméo Relay (1.0)
tf	358.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.93	J/mol×K	562.92	Joback Method

cpg	276.15	J/mol×K	601.37	Joback Method
cpg	286.68	J/mol×K	639.83	Joback Method
cpg	296.53	J/mol×K	678.28	Joback Method
cpg	305.72	J/mol×K	716.73	Joback Method
cpg	314.25	J/mol×K	755.19	Joback Method
cpg	322.15	J/mol×K	793.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2439772&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The thermodynamic stability of the three isomers of methoxybenzamide: An experimental and computational study:	https://www.doi.org/10.1016/j.jct.2013.06.022

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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