

Propanamide, N-(4-methoxyphenyl)-2-bromo-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C10H12BrNO2/c1-7(11)10(13)12-8-3-5-9(14-2)6-4-8/h3-7H,1-2H3,(H,12,13)

OHKOKTSMJKGAHR-UHFFFAOYSA-N

C10H12BrNO2

COc1ccc(NC(=O)C(C)Br)cc1

258.11

Physical Properties

Property code	Value	Unit	Source
gf	3.45	kJ/mol	Joback Method
hf	-194.95	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.417		Crippen Method
mcvol	162.920	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	652.04	K	Joback Method
tc	882.30	K	Joback Method
tf	411.02	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.44	J/mol×K	652.04	Joback Method
cpg	396.83	J/mol×K	690.42	Joback Method
cpg	408.35	J/mol×K	728.79	Joback Method
cpg	419.04	J/mol×K	767.17	Joback Method
cpg	428.93	J/mol×K	805.55	Joback Method
cpg	438.03	J/mol×K	843.93	Joback Method
cpg	446.39	J/mol×K	882.30	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=U307476&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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