Propanamide, N-(2,5-dimethoxyphenyl)-2-bromo-

Inchi: InChI=1S/C11H14BrNO3/c1-7(12)11(14)13-9-6-8(15-2)4-5-10(9)16-3/h4-7H,1-3H3,(H,13

InchiKey: YSRWCGOGVBPWOI-UHFFFAOYSA-N

Formula: C11H14BrNO3

SMILES: COc1ccc(OC)c(NC(=O)C(C)Br)c1

Mol. weight [g/mol]: 288.14

Physical Properties

Property code	Value	Unit	Source
gf	-102.76	kJ/mol	Joback Method
hf	-359.28	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	67.73	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.426		Crippen Method
mcvol	182.880	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1932.00		NIST Webbook
tb	702.32	K	Joback Method
tc	926.19	K	Joback Method
tf	457.04	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.44	J/mol×K	702.32	Joback Method
cpg	470.08	J/mol×K	739.63	Joback Method
cpg	481.86	J/mol×K	776.94	Joback Method
cpg	492.78	J/mol×K	814.25	Joback Method
cpg	502.86	J/mol×K	851.57	Joback Method
cpg	512.11	J/mol×K	888.88	Joback Method
cpg	520.52	J/mol×K	926.19	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=U307478&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume