Propanoic acid, 2-dimethylamino-3-(4-methoxyphenyl), methyl ester

Inchi: InChI=1S/C13H19NO3/c1-14(2)12(13(15)17-4)9-10-5-7-11(16-3)8-6-10/h5-8,12H,9H2,1-

InchiKey: VIFCXBHBJYGIIQ-UHFFFAOYSA-N

Formula: C13H19NO3

SMILES: COC(=O)C(Cc1ccc(OC)cc1)N(C)C

Mol. weight [g/mol]: 237.29

Physical Properties

Property code	Value	Unit	Source
gf	-69.22	kJ/mol	Joback Method
hf	-401.36	kJ/mol	Joback Method
hfus	26.55	kJ/mol	Joback Method
hvap	60.69	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.341		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	1690.00		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	639.21	K	Joback Method
tc	842.43	K	Joback Method
tf	387.07	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.90	J/mol×K	639.21	Joback Method
cpg	523.84	J/mol×K	673.08	Joback Method
cpg	538.86	J/mol×K	706.95	Joback Method
cpg	552.99	J/mol×K	740.82	Joback Method
cpg	566.24	J/mol×K	774.69	Joback Method
cpg	578.63	J/mol×K	808.56	Joback Method
cpg	590.16	J/mol×K	842.43	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=R106733&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