3,4,5-Trimethoxybenzyl methylamine

Inchi: InChI=1S/C11H17NO3/c1-12-7-8-5-9(13-2)11(15-4)10(6-8)14-3/h5-6,12H,7H2,1-4H3
InchiKey: LFULMNRPABTDDQ-UHFFFAOYSA-N
Formula: C11H17NO3
SMILES: CNCc1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]: 211.26
CAS: 58780-82-8

Physical Properties

Property code	Value	Unit	Source
gf	-100.35	kJ/mol	Joback Method
hf	-411.44	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.432		Crippen Method
mcvol	169.680	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	610.13	K	Joback Method
tc	810.87	K	Joback Method
tf	397.06	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.17	J/mol×K	610.13	Joback Method
cpg	441.52	J/mol×K	643.59	Joback Method
cpg	455.24	J/mol×K	677.04	Joback Method
cpg	468.31	J/mol×K	710.50	Joback Method
cpg	480.72	J/mol×K	743.95	Joback Method
cpg	492.44	J/mol×K	777.41	Joback Method
cpg	503.45	J/mol×K	810.87	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=C58780828&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