Methyl(n-cyanomethyl-n-benzyl)-beta-aminopropi

Inchi: InChI=1S/C13H16N2O2/c1-17-13(16)7-9-15(10-8-14)11-12-5-3-2-4-6-12/h2-6H,7,9-11H2
InchiKey: UMSPRCKJZSNNFN-UHFFFAOYSA-N
Formula: C13H16N2O2
SMILES: COC(=O)CCN(CC#N)Cc1ccccc1
Mol. weight [g/mol]: 232.28
CAS: 116558-09-9

Physical Properties

Property code	Value	Unit	Source
gf	181.03	kJ/mol	Joback Method
hf	-87.51	kJ/mol	Joback Method
hfus	30.78	kJ/mol	Joback Method
hvap	68.48	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.575		Crippen Method
mcvol	189.070	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
tb	714.33	K	Joback Method
tc	927.62	K	Joback Method
tf	432.31	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.26	J/mol×K	714.33	Joback Method
cpg	524.43	J/mol×K	749.88	Joback Method
cpg	536.70	J/mol×K	785.43	Joback Method
cpg	548.10	J/mol×K	820.98	Joback Method
cpg	558.65	J/mol×K	856.53	Joback Method
cpg	568.41	J/mol×K	892.08	Joback Method
cpg	577.41	J/mol×K	927.62	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=C116558099&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