Methyl-beta-benzylamino propionate

Inchi: InChI=1S/C11H15NO2/c1-14-11(13)7-8-12-9-10-5-3-2-4-6-10/h2-6,12H,7-9H2,1H3
InchiKey: MVZIUHUSHIYYGP-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: COC(=O)CCNCc1ccccc1
Mol. weight [g/mol]: 193.24
CAS: 23574-01-8

Physical Properties

Property code	Value	Unit	Source
gf	9.62	kJ/mol	Joback Method
hf	-225.17	kJ/mol	Joback Method
hfus	26.17	kJ/mol	Joback Method
hvap	57.95	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.339		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	604.22	K	Joback Method
tc	813.47	K	Joback Method
tf	364.97	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.32	J/mol×K	604.22	Joback Method
cpg	410.59	J/mol×K	639.10	Joback Method
cpg	424.01	J/mol×K	673.97	Joback Method
cpg	436.60	J/mol×K	708.85	Joback Method
cpg	448.39	J/mol×K	743.72	Joback Method
cpg	459.41	J/mol×K	778.60	Joback Method
cpg	469.67	J/mol×K	813.47	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=C23574018&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

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