methantheline

Inchi: InChI=1S/C20H23NO3/c1-3-21(4-2)13-14-23-20(22)19-15-9-5-7-11-17(15)24-18-12-8-6-
InchiKey: HIGMQFBAGGGECD-UHFFFAOYSA-N
Formula: C20H23NO3
SMILES: CCN(CC)CCOC(=O)C1c2ccccc2Oc2ccccc21
Mol. weight [g/mol]: 325.40
CAS: 5818-17-7

Physical Properties

Property code	Value	Unit	Source
gf	186.67	kJ/mol	Joback Method
hf	-236.32	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.809		Crippen Method
mcvol	257.570	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2283.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	838.47	K	Joback Method
tc	1060.69	K	Joback Method
tf	545.70	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.00	J/mol×K	838.47	Joback Method
cpg	805.63	J/mol×K	875.51	Joback Method
cpg	820.21	J/mol×K	912.54	Joback Method
cpg	833.84	J/mol×K	949.58	Joback Method
cpg	846.62	J/mol×K	986.61	Joback Method
cpg	858.64	J/mol×K	1023.65	Joback Method

cpg	870.01	J/mol×K	1060.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5818177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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