Putrescine, bis-isoBOC

Inchi: InChI=1S/C14H28N2O4/c1-11(2)9-19-13(17)15-7-5-6-8-16-14(18)20-10-12(3)4/h11-12H
InchiKey: YVGVGACZXWMVSU-UHFFFAOYSA-N
Formula: C14H28N2O4
SMILES: CC(C)COC(=O)NCCCCNC(=O)OCC(C)C
Mol. weight [g/mol]: 288.38

Physical Properties

Property code	Value	Unit	Source
gf	-226.94	kJ/mol	Joback Method
hf	-725.51	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	77.17	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.531		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	2154.00		NIST Webbook
tb	771.76	K	Joback Method
tc	959.40	K	Joback Method
tf	467.18	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.77	J/mol×K	771.76	Joback Method
cpg	756.03	J/mol×K	803.03	Joback Method
cpg	770.38	J/mol×K	834.31	Joback Method
cpg	783.82	J/mol×K	865.58	Joback Method
cpg	796.36	J/mol×K	896.85	Joback Method
cpg	808.02	J/mol×K	928.13	Joback Method
cpg	818.80	J/mol×K	959.40	Joback Method

Sources

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=R392815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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