1,3-Diaminopropane, bis-isoBOC

Inchi: InChI=1S/C13H26N2O4/c1-10(2)8-18-12(16)14-6-5-7-15-13(17)19-9-11(3)4/h10-11H,5-9
InchiKey: ABAUDNZDYWBCOE-UHFFFAOYSA-N
Formula: C13H26N2O4
SMILES: CC(C)COC(=O)NCCCNC(=O)OCC(C)C
Mol. weight [g/mol]: 274.36

Physical Properties

Property code	Value	Unit	Source
gf	-235.36	kJ/mol	Joback Method
hf	-704.87	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	74.94	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.141		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	748.88	K	Joback Method
tc	936.27	K	Joback Method
tf	455.91	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.30	J/mol×K	748.88	Joback Method
cpg	699.19	J/mol×K	780.11	Joback Method
cpg	713.22	J/mol×K	811.34	Joback Method
cpg	726.39	J/mol×K	842.58	Joback Method
cpg	738.70	J/mol×K	873.81	Joback Method
cpg	750.17	J/mol×K	905.04	Joback Method
cpg	760.80	J/mol×K	936.27	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392335&Units=SI

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