Diambutol

Inchi: InChI=1S/C10H24N2O2/c1-3-9(7-13)11-5-6-12-10(4-2)8-14/h9-14H,3-8H2,1-2H3
InchiKey: AEUTYOVWOVBAKS-UHFFFAOYSA-N
Formula: C10H24N2O2
SMILES: CCC(CO)NCCNC(CC)CO
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	-66.42	kJ/mol	Joback Method
hf	-457.81	kJ/mol	Joback Method
hfus	32.98	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Joback Method
log10ws	-0.56		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.293		Crippen Method
mcvol	183.460	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	712.02	K	Joback Method
tc	882.71	K	Joback Method
tf	399.42	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.21	J/mol×K	712.02	Joback Method
cpg	561.30	J/mol×K	740.47	Joback Method
cpg	572.81	J/mol×K	768.92	Joback Method
cpg	583.77	J/mol×K	797.37	Joback Method
cpg	594.18	J/mol×K	825.82	Joback Method
cpg	604.08	J/mol×K	854.27	Joback Method
cpg	613.48	J/mol×K	882.71	Joback Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume