Metabutethamine

Inchi: InChI=1S/C13H20N2O2/c1-10(2)9-15-6-7-17-13(16)11-4-3-5-12(14)8-11/h3-5,8,10,15H,6
InchiKey: BXMFKNRZTLNAFY-UHFFFAOYSA-N
Formula: C13H20N2O2
SMILES: CC(C)CNCCOC(=O)c1cccc(N)c1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	80.84	kJ/mol	Joback Method
hf	-249.41	kJ/mol	Joback Method
hfus	32.64	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.671		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1988.00		NIST Webbook
rinpol	1988.00		NIST Webbook
tb	727.05	K	Joback Method
tc	941.53	K	Joback Method
tf	468.29	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.24	J/mol×K	727.05	Joback Method
cpg	575.84	J/mol×K	762.80	Joback Method
cpg	589.47	J/mol×K	798.54	Joback Method
cpg	602.15	J/mol×K	834.29	Joback Method
cpg	613.91	J/mol×K	870.04	Joback Method
cpg	624.78	J/mol×K	905.78	Joback Method
cpg	634.78	J/mol×K	941.53	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=R18062&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