Phenetamine

Other names: Feclemine
Inchi: InChI=1S/C24H42N2/c1-5-25(6-2)19-23(20-26(7-3)8-4)24(21-15-11-9-12-16-21)22-17-13
InchiKey: QDMORDTWFMWOFA-UHFFFAOYSA-N
Formula: C24H42N2
SMILES: CCN(CC)CC(CN(CC)CC)C(c1ccccc1)C1CCCCC1
Mol. weight [g/mol]: 358.60
CAS: 3590-16-7

Physical Properties

Property code	Value	Unit	Source
gf	504.74	kJ/mol	Joback Method
hf	-123.34	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	75.03	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.650		Crippen Method
mcvol	334.360	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	818.75	K	Joback Method
tc	1023.09	K	Joback Method
tf	428.98	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.31	J/mol×K	818.75	Joback Method
cpg	1118.22	J/mol×K	852.81	Joback Method
cpg	1139.64	J/mol×K	886.86	Joback Method
cpg	1159.65	J/mol×K	920.92	Joback Method

cpg	1178.34	J/mol×K	954.98	Joback Method
cpg	1195.82	J/mol×K	989.04	Joback Method
cpg	1212.16	J/mol×K	1023.09	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=C3590167&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