Lefetamine

Inchi: InChI=1S/C16H19N/c1-14(2)17(16-11-7-4-8-12-16)13-15-9-5-3-6-10-15/h3-12,14H,13H2
InchiKey: OJKDJKUSLNKNEL-UHFFFAOYSA-N
Formula: C16H19N
SMILES: CC(C)N(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 225.33
CAS: 7262-75-1

Physical Properties

Property code	Value	Unit	Source
gf	417.00	kJ/mol	Joback Method
hf	161.74	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	57.42	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.102		Crippen Method
mcvol	198.760	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1670.00		NIST Webbook
tb	630.84	K	Joback Method
tc	862.00	K	Joback Method
tf	340.39	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.02	J/mol×K	630.84	Joback Method
cpg	530.37	J/mol×K	669.37	Joback Method
cpg	548.26	J/mol×K	707.89	Joback Method
cpg	564.80	J/mol×K	746.42	Joback Method
cpg	580.07	J/mol×K	784.95	Joback Method
cpg	594.17	J/mol×K	823.47	Joback Method
cpg	607.18	J/mol×K	862.00	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=C7262751&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