1-(N-Benzyl-N-butanoyl)amino-6-(2-cycnoethyl)cy

Inchi: InChI=1S/C20H26N2O/c1-2-9-20(23)22(16-17-10-4-3-5-11-17)19-14-7-6-12-18(19)13-8-
InchiKey: NPUTWCIUHVADOH-UHFFFAOYSA-N
Formula: C20H26N2O
SMILES: CCCC(=O)N(Cc1ccccc1)C1=CCCCC1CCC#N
Mol. weight [g/mol]: 310.43
CAS: 85019-63-2

Physical Properties

Property code	Value	Unit	Source
gf	389.75	kJ/mol	Joback Method
hf	0.86	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.803		Crippen Method
mcvol	266.670	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
tb	875.76	K	Joback Method
tc	1102.30	K	Joback Method
tf	509.63	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.31	J/mol×K	875.76	Joback Method
cpg	855.16	J/mol×K	913.52	Joback Method
cpg	869.75	J/mol×K	951.27	Joback Method
cpg	883.19	J/mol×K	989.03	Joback Method
cpg	895.54	J/mol×K	1026.79	Joback Method
cpg	906.90	J/mol×K	1064.54	Joback Method
cpg	917.35	J/mol×K	1102.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85019632&Units=SI
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

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