1-(N-Benzyl-N-pentanoyl)amino-6-(2-cyanoethyl)c

Inchi: InChI=1S/C21H28N2O/c1-2-3-15-21(24)23(17-18-10-5-4-6-11-18)20-14-8-7-12-19(20)13

InchiKey: DJCCMGJAIYGHMH-UHFFFAOYSA-N

Formula: C21H28N2O

SMILES: CCCCC(=O)N(Cc1ccccc1)C1=CCCCC1CCC#N

Mol. weight [g/mol]: 324.46

CAS: 85031-41-0

Physical Properties

Property code	Value	Unit	Source
gf	398.17	kJ/mol	Joback Method
hf	-19.78	kJ/mol	Joback Method
hfus	42.98	kJ/mol	Joback Method
hvap	85.27	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.193		Crippen Method
mcvol	280.760	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
tb	898.64	K	Joback Method
tc	1123.61	K	Joback Method
tf	520.90	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.23	J/mol×K	898.64	Joback Method
cpg	914.16	J/mol×K	936.14	Joback Method
cpg	928.84	J/mol×K	973.63	Joback Method
cpg	942.38	J/mol×K	1011.13	Joback Method
cpg	954.84	J/mol×K	1048.62	Joback Method
cpg	966.33	J/mol×K	1086.12	Joback Method
cpg	976.92	J/mol×K	1123.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85031410&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

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