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

Inchi: InChI=1S/C20H26N2O/c1-16(2)20(23)22(15-17-9-4-3-5-10-17)19-13-7-6-11-18(19)12-8-
InchiKey: QWWSKVKYJQRAHH-UHFFFAOYSA-N
Formula: C20H26N2O
SMILES: CC(C)C(=O)N(Cc1ccccc1)C1=CCCCC1CCC#N
Mol. weight [g/mol]: 310.43
CAS: 85019-65-4

Physical Properties

Property code	Value	Unit	Source
gf	387.31	kJ/mol	Joback Method
hf	-4.42	kJ/mol	Joback Method
hfus	36.87	kJ/mol	Joback Method
hvap	82.65	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.659		Crippen Method
mcvol	266.670	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
tb	875.32	K	Joback Method
tc	1104.85	K	Joback Method
tf	494.63	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.83	J/mol×K	875.32	Joback Method
cpg	855.86	J/mol×K	913.58	Joback Method
cpg	870.58	J/mol×K	951.83	Joback Method
cpg	884.10	J/mol×K	990.09	Joback Method
cpg	896.51	J/mol×K	1028.34	Joback Method
cpg	907.88	J/mol×K	1066.60	Joback Method
cpg	918.31	J/mol×K	1104.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85019654&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