1-(N-Benzyl-N-3-methylbutanoyl)amino-6-(2-cyano

Inchi: InChI=1S/C21H28N2O/c1-17(2)15-21(24)23(16-18-9-4-3-5-10-18)20-13-7-6-11-19(20)12
InchiKey: LTQZBXHZGZZBRE-UHFFFAOYSA-N
Formula: C21H28N2O
SMILES: CC(C)CC(=O)N(Cc1ccccc1)C1=CCCCC1CCC#N
Mol. weight [g/mol]: 324.46
CAS: 85019-64-3

Physical Properties

Property code	Value	Unit	Source
gf	395.73	kJ/mol	Joback Method
hf	-25.06	kJ/mol	Joback Method
hfus	39.46	kJ/mol	Joback Method
hvap	84.88	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.049		Crippen Method
mcvol	280.760	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
tb	898.20	K	Joback Method
tc	1125.82	K	Joback Method
tf	505.90	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.73	J/mol×K	898.20	Joback Method
cpg	914.81	J/mol×K	936.14	Joback Method
cpg	929.60	J/mol×K	974.07	Joback Method
cpg	943.20	J/mol×K	1012.01	Joback Method
cpg	955.69	J/mol×K	1049.95	Joback Method
cpg	967.17	J/mol×K	1087.88	Joback Method
cpg	977.73	J/mol×K	1125.82	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=C85019643&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume