1-Buten-3-one, 1-(benzylamino)-

Inchi: InChI=1S/C11H13NO/c1-10(13)7-8-12-9-11-5-3-2-4-6-11/h2-8,12H,9H2,1H3/b8-7+
InchiKey: CQWWYPKMJPSBJK-BQYQJAHWSA-N
Formula: C11H13NO
SMILES: CC(=O)C=CNCc1ccccc1
Mol. weight [g/mol]: 175.23
CAS: 53133-41-8

Physical Properties

Property code	Value	Unit	Source
gf	194.84	kJ/mol	Joback Method
hf	24.27	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	55.50	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	1.879		Crippen Method
mcvol	149.340	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	585.96	K	Joback Method
tc	806.81	K	Joback Method
tf	337.66	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.25	J/mol×K	585.96	Joback Method
cpg	365.28	J/mol×K	622.77	Joback Method
cpg	378.34	J/mol×K	659.58	Joback Method
cpg	390.50	J/mol×K	696.39	Joback Method
cpg	401.80	J/mol×K	733.19	Joback Method
cpg	412.31	J/mol×K	770.00	Joback Method
cpg	422.08	J/mol×K	806.81	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=C53133418&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