3-(Benzylmethylamino)-1-propanol

Other names: 1-Propanol, 3-[methyl(phenylmethyl)amino]-
3-(N-benzyl-N-methylamino)propan-1-ol
Inchi: InChI=1S/C11H17NO/c1-12(8-5-9-13)10-11-6-3-2-4-7-11/h2-4,6-7,13H,5,8-10H2,1H3
InchiKey: YQAUZGVTGQVMPM-UHFFFAOYSA-N
Formula: C11H17NO
SMILES: CN(CCCO)Cc1ccccc1
Mol. weight [g/mol]: 179.26
CAS: 5814-42-6

Physical Properties

Property code	Value	Unit	Source
gf	128.11	kJ/mol	Joback Method
hf	-118.54	kJ/mol	Joback Method
hfus	25.40	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.501		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	582.38	K	Joback Method
tc	770.30	K	Joback Method
tf	333.44	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.44	J/mol×K	582.38	Joback Method
cpg	408.18	J/mol×K	613.70	Joback Method
cpg	421.14	J/mol×K	645.02	Joback Method
cpg	433.37	J/mol×K	676.34	Joback Method
cpg	444.89	J/mol×K	707.66	Joback Method
cpg	455.75	J/mol×K	738.98	Joback Method
cpg	465.97	J/mol×K	770.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.70	K	0.50	NIST Webbook

Sources

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=C5814426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume