Benzylcarbamate

Other names:	Carbamic acid benzyl ester
	Carbamic acid, phenylmethyl ester
	o-benzyl carbamate
Inchi:	InChI=1S/C8H9NO2/c9-8(10)11-6-7-4-2-1-3-5-7/h1-5H,6H2,(H2,9,10)
InchiKey:	PUJDIJCNWFYVJX-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	NC(=O)OCc1ccccc1
Mol. weight [g/mol]:	151.16
CAS:	621-84-1

Physical Properties

Property code	Value	Unit	Source
gf	-38.58	kJ/mol	Joback Method
hf	-182.93	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	55.47	kJ/mol	Joback Method
log10ws	-0.35		Aqueous Solubility Prediction Method
logp	1.282		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	557.94	K	Joback Method
tc	787.57	K	Joback Method
tf	360.65	K	Aqueous Solubility Prediction Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.77	J/mol×K	557.94	Joback Method
cpg	277.29	J/mol×K	596.21	Joback Method
cpg	288.07	J/mol×K	634.48	Joback Method
cpg	298.11	J/mol×K	672.75	Joback Method

cpg	307.45	J/mol×K	711.03	Joback Method
cpg	316.09	J/mol×K	749.30	Joback Method
cpg	324.07	J/mol×K	787.57	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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