Isobutylcarbamate, N-(2-phenylethyl)

Inchi: InChI=1S/C13H19NO2/c1-11(2)10-16-13(15)14-9-8-12-6-4-3-5-7-12/h3-7,11H,8-10H2,1-
InchiKey: AHJFRWJXEBIIQT-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CC(C)COC(=O)NCCc1ccccc1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	24.02	kJ/mol	Joback Method
hf	-271.73	kJ/mol	Joback Method
hfus	27.83	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.611		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	649.54	K	Joback Method
tc	856.42	K	Joback Method
tf	372.51	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.58	J/mol×K	649.54	Joback Method
cpg	513.29	J/mol×K	684.02	Joback Method
cpg	528.04	J/mol×K	718.50	Joback Method
cpg	541.86	J/mol×K	752.98	Joback Method
cpg	554.79	J/mol×K	787.46	Joback Method
cpg	566.86	J/mol×K	821.94	Joback Method
cpg	578.08	J/mol×K	856.42	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=R392508&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume