Carbamic acid, 3-methylphenyl-, isobutyl ester

Other names: Isobutylcarbamate, N-(3-methylphenyl)
Inchi: InChI=1S/C12H17NO2/c1-9(2)8-15-12(14)13-11-6-4-5-10(3)7-11/h4-7,9H,8H2,1-3H3,(H,
InchiKey: MXLDHGQMNSRKFX-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: Cc1cccc(NC(=O)OCC(C)C)c1
Mol. weight [g/mol]: 207.27

Physical Properties

Property code	Value	Unit	Source
gf	5.97	kJ/mol	Joback Method
hf	-262.56	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.200		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	631.64	K	Joback Method
tc	842.61	K	Joback Method
tf	373.76	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.86	J/mol×K	631.64	Joback Method
cpg	460.85	J/mol×K	666.80	Joback Method
cpg	474.96	J/mol×K	701.96	Joback Method
cpg	488.20	J/mol×K	737.13	Joback Method
cpg	500.60	J/mol×K	772.29	Joback Method
cpg	512.17	J/mol×K	807.45	Joback Method
cpg	522.93	J/mol×K	842.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U314741&Units=SI
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

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