Carbamic acid, 2,4-dimethylphenyl, butyl ester

Inchi: InChI=1S/C13H19NO2/c1-4-5-8-16-13(15)14-12-7-6-10(2)9-11(12)3/h6-7,9H,4-5,8H2,1-3
InchiKey: JRICEOSBCKGWME-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCCCOC(=O)Nc1ccc(C)cc1C
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	7.20	kJ/mol	Joback Method
hf	-289.39	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.652		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	659.94	K	Joback Method
tc	864.79	K	Joback Method
tf	412.55	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.91	J/mol×K	659.94	Joback Method
cpg	510.94	J/mol×K	694.08	Joback Method
cpg	525.13	J/mol×K	728.22	Joback Method
cpg	538.49	J/mol×K	762.37	Joback Method
cpg	551.03	J/mol×K	796.51	Joback Method
cpg	562.78	J/mol×K	830.65	Joback Method
cpg	573.75	J/mol×K	864.79	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=R37709&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