Isobutyl 2-(isobutoxycarbonyloxy)ethylcarbamate

Inchi: InChI=1S/C12H23NO5/c1-9(2)7-17-11(14)13-5-6-16-12(15)18-8-10(3)4/h9-10H,5-8H2,1-

InchiKey: CWJBVYLJEKSWIV-UHFFFAOYSA-N

Formula: C12H23NO5

SMILES: CC(C)COC(=O)NCCOC(=O)OCC(C)C

Mol. weight [g/mol]: 261.31

Physical Properties

Property code	Value	Unit	Source
gf	-438.17	kJ/mol	Joback Method
hf	-869.92	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	68.69	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.178		Crippen Method
mcvol	210.670	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1748.00		NIST Webbook
tb	698.25	K	Joback Method
tc	883.16	K	Joback Method
tf	414.21	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.31	J/mol×K	698.25	Joback Method
cpg	614.96	J/mol×K	729.07	Joback Method
cpg	628.85	J/mol×K	759.89	Joback Method
cpg	641.96	J/mol×K	790.70	Joback Method
cpg	654.28	J/mol×K	821.52	Joback Method
cpg	665.82	J/mol×K	852.34	Joback Method
cpg	676.56	J/mol×K	883.16	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=U373682&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