1,2-Butanediol, 2-phenyl-, 1-carbamate

Inchi: InChI=1S/C11H15NO3/c1-2-11(14,8-15-10(12)13)9-6-4-3-5-7-9/h3-7,14H,2,8H2,1H3,(H2
InchiKey: WAFIYOULDIWAKR-UHFFFAOYSA-N
Formula: C11H15NO3
SMILES: CCC(O)(COC(N)=O)c1ccccc1
Mol. weight [g/mol]: 209.25

Physical Properties

Property code	Value	Unit	Source
hfus	22.94	kJ/mol	Joback Method
log10ws	-1.46		Cheméo Relay (1.0)
logp	1.380		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
tf	347.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.80	J/mol×K	715.53	Joback Method
cpg	472.28	J/mol×K	751.07	Joback Method
cpg	482.92	J/mol×K	786.61	Joback Method
cpg	492.77	J/mol×K	822.15	Joback Method
cpg	501.89	J/mol×K	857.69	Joback Method
cpg	510.31	J/mol×K	893.23	Joback Method
cpg	518.09	J/mol×K	928.77	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50191&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point