Felbamate

Other names:	1,3-Propanediol, 2-phenyl-, dicarbamate
	2-Phenyl-1,3-propanediol dicarbamate
	ADD-03055
	Felbamyl
	Felbatol
	Taloxa
	W-554
	2-phenylpropane-1,3-diyl dicarbamate
Inchi:	InChI=1S/C11H14N2O4/c12-10(14)16-6-9(7-17-11(13)15)8-4-2-1-3-5-8/h1-5,9H,6-7H2,(H
InchiKey:	WKGXYQFOCVYPAC-UHFFFAOYSA-N
Formula:	C11H14N2O4
SMILES:	NC(=O)OCC(COC(N)=O)c1ccccc1
Mol. weight [g/mol]:	238.24
CAS:	25451-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-183.23	kJ/mol	Joback Method
hf	-461.14	kJ/mol	Joback Method
hfus	30.73	kJ/mol	Joback Method
hvap	81.56	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	0.961		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	2157.00		NIST Webbook
tb	774.96	K	Joback Method
tc	1005.57	K	Joback Method
tf	535.99	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	502.87	J/mol×K	774.96	Joback Method
cpg	514.32	J/mol×K	813.40	Joback Method
cpg	524.76	J/mol×K	851.83	Joback Method
cpg	534.21	J/mol×K	890.27	Joback Method
cpg	542.67	J/mol×K	928.70	Joback Method
cpg	550.17	J/mol×K	967.14	Joback Method
cpg	556.71	J/mol×K	1005.57	Joback Method

Sources

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=C25451154&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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