Propane, 1,3-bis-(methoxycarbonylamino)

Inchi: InChI=1S/C7H14N2O4/c1-12-6(10)8-4-3-5-9-7(11)13-2/h3-5H2,1-2H3,(H,8,10)(H,9,11)
InchiKey: KPPQHGGHTCGGOK-UHFFFAOYSA-N
Formula: C7H14N2O4
SMILES: COC(=O)NCCCNC(=O)OC
Mol. weight [g/mol]: 190.20

Physical Properties

Property code	Value	Unit	Source
gf	-281.00	kJ/mol	Joback Method
hf	-570.47	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	62.36	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.089		Crippen Method
mcvol	144.330	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1485.00		NIST Webbook
tb	612.48	K	Joback Method
tc	801.29	K	Joback Method
tf	418.29	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.08	J/mol×K	612.48	Joback Method
cpg	381.19	J/mol×K	643.95	Joback Method
cpg	391.79	J/mol×K	675.42	Joback Method
cpg	401.86	J/mol×K	706.89	Joback Method
cpg	411.40	J/mol×K	738.35	Joback Method
cpg	420.40	J/mol×K	769.82	Joback Method
cpg	428.85	J/mol×K	801.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333727&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