

Pentane, 1,5-bis-(methoxycarbonylamino)

Inchi:

GLRSKDCBNNEWJE-UHFFFAOYSA-N

InchiKey:

C9H18N2O4

Formula:

COC(=O)NCCCCCNC(=O)OC

SMILES:

218.25

Mol. weight [g/mol]:

Physical Properties

Property code	Value	Unit	Source
gf	-264.16	kJ/mol	Joback Method
hf	-611.75	kJ/mol	Joback Method
hfus	34.84	kJ/mol	Joback Method
hvap	66.81	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	0.869		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1727.00		NIST Webbook
tb	658.24	K	Joback Method
tc	843.63	K	Joback Method
tf	440.83	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.96	J/mol×K	658.24	Joback Method
cpg	481.48	J/mol×K	689.14	Joback Method
cpg	493.37	J/mol×K	720.04	Joback Method
cpg	504.64	J/mol×K	750.93	Joback Method
cpg	515.29	J/mol×K	781.83	Joback Method
cpg	525.30	J/mol×K	812.73	Joback Method
cpg	534.69	J/mol×K	843.63	Joback Method

Sources

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=R333712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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