Butane, 1,4-bis-(methoxycarbonylamino)

Inchi: InChI=1S/C8H16N2O4/c1-13-7(11)9-5-3-4-6-10-8(12)14-2/h3-6H2,1-2H3,(H,9,11)(H,10,1
InchiKey: OQNSLWFDULDLQM-UHFFFAOYSA-N
Formula: C8H16N2O4
SMILES: COC(=O)NCCCCNC(=O)OC
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
gf	-272.58	kJ/mol	Joback Method
hf	-591.11	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	64.59	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	0.479		Crippen Method
mcvol	158.420	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1622.00		NIST Webbook
tb	635.36	K	Joback Method
tc	822.30	K	Joback Method
tf	429.56	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.75	J/mol×K	635.36	Joback Method
cpg	430.61	J/mol×K	666.52	Joback Method
cpg	441.89	J/mol×K	697.67	Joback Method
cpg	452.60	J/mol×K	728.83	Joback Method
cpg	462.73	J/mol×K	759.99	Joback Method
cpg	472.28	J/mol×K	791.14	Joback Method
cpg	481.24	J/mol×K	822.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333658&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