(3S,6S)-3-Butyl-6-methylpiperazine-2,5-dione

Inchi: InChI=1S/C9H16N2O2/c1-3-4-5-7-9(13)10-6(2)8(12)11-7/h6-7H,3-5H2,1-2H3,(H,10,13)(H
InchiKey: SHYWDFCZXCPLHM-UHFFFAOYSA-N
Formula: C9H16N2O2
SMILES: CCCCC1NC(=O)C(C)NC1=O
Mol. weight [g/mol]: 184.24

Physical Properties

Property code	Value	Unit	Source
gf	-28.12	kJ/mol	Joback Method
hf	-394.89	kJ/mol	Joback Method
hfus	30.17	kJ/mol	Joback Method
hvap	57.76	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	0.180		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	652.94	K	Joback Method
tc	891.42	K	Joback Method
tf	540.83	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.17	J/mol×K	652.94	Joback Method
cpg	436.38	J/mol×K	692.69	Joback Method
cpg	453.55	J/mol×K	732.43	Joback Method
cpg	469.61	J/mol×K	772.18	Joback Method
cpg	484.47	J/mol×K	811.92	Joback Method
cpg	498.05	J/mol×K	851.67	Joback Method
cpg	510.27	J/mol×K	891.42	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=U375959&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