3-Carbethoxy-2,5-piperazinedione

Inchi: InChI=1S/C7H10N2O4/c1-2-13-7(12)5-6(11)8-3-4(10)9-5/h5H,2-3H2,1H3,(H,8,11)(H,9,1
InchiKey: JGDBWGPIUGDQTO-UHFFFAOYSA-N
Formula: C7H10N2O4
SMILES: CCOC(=O)C1NC(=O)CNC1=O
Mol. weight [g/mol]: 186.17
CAS: 86750-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-271.17	kJ/mol	Joback Method
hf	-578.07	kJ/mol	Joback Method
hfus	26.71	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	0.45		Crippen Method
logp	-1.836		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	688.14	K	Joback Method
tc	938.95	K	Joback Method
tf	594.69	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.14	J/mol×K	688.14	Joback Method
cpg	369.76	J/mol×K	729.94	Joback Method
cpg	383.33	J/mol×K	771.74	Joback Method
cpg	395.74	J/mol×K	813.55	Joback Method
cpg	406.87	J/mol×K	855.35	Joback Method
cpg	416.59	J/mol×K	897.15	Joback Method
cpg	424.78	J/mol×K	938.95	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=C86750347&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume