2,5-Piperazinedione, 3-methyl-6-(1-methylethyl)-

Other names: 3-methyl-6-(1-methylethyl)-2,5-piperazinedione
Inchi: InChI=1S/C8H14N2O2/c1-4(2)6-8(12)9-5(3)7(11)10-6/h4-6H,1-3H3,(H,9,12)(H,10,11)
InchiKey: ORLDMMKUTCCBSM-UHFFFAOYSA-N
Formula: C8H14N2O2
SMILES: CC1NC(=O)C(C(C)C)NC1=O
Mol. weight [g/mol]: 170.21
CAS: 22160-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-38.98	kJ/mol	Joback Method
hf	-379.53	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	55.14	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	-0.355		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	629.62	K	Joback Method
tc	878.66	K	Joback Method
tf	514.56	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.38	J/mol×K	629.62	Joback Method
cpg	385.38	J/mol×K	671.13	Joback Method
cpg	402.39	J/mol×K	712.63	Joback Method
cpg	418.32	J/mol×K	754.14	Joback Method
cpg	433.05	J/mol×K	795.64	Joback Method
cpg	446.50	J/mol×K	837.15	Joback Method
cpg	458.58	J/mol×K	878.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22160425&Units=SI

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