

2,5 Piperazinedione, 3,6-bis(1-methylethyl)-, (3S)-trans-

Inchi:	InChI=1S/C10H18N2O2/c1-5(2)7-9(13)12-8(6(3)4)10(14)11-7/h5-8H,1-4H3,(H,11,14)(H,
InchiKey:	QGMAWEIDGADSAC-OCAPTIKFSA-N
Formula:	C10H18N2O2
SMILES:	CC(C)C1NC(=O)C(C(C)C)NC1=O
Mol. weight [g/mol]:	198.26
CAS:	19943-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-24.58	kJ/mol	Joback Method
hf	-426.09	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	59.21	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	0.282		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	674.94	K	Joback Method
tc	918.34	K	Joback Method
tf	522.10	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.86	J/molxK	674.94	Joback Method
cpg	491.41	J/molxK	715.51	Joback Method
cpg	509.71	J/molxK	756.07	Joback Method
cpg	526.67	J/molxK	796.64	Joback Method
cpg	542.22	J/molxK	837.21	Joback Method
cpg	556.27	J/molxK	877.78	Joback Method
cpg	568.75	J/molxK	918.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C19943147&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

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