

4,6-Ethano-1h,8h-pyrano[3,4-c]pyran-1,8-dione, hexahydro-3,3,6-trimethyl-8a-[2-(dimethylamino)]e

Inchi: CN(C)CCC12C(=O)OC3(C)CCC(C1C3)C(C)(C)OC2=O
InchiKey: ICQWUTZYWRVNMN-UHFFFAOYSA-N
Formula: C17H27NO4
SMILES: CN(C)CCC12C(=O)OC3(C)CCC(C1C3)C(C)(C)OC2=O
Mol. weight [g/mol]: 309.40

Physical Properties

Property code	Value	Unit	Source
gf	-100.32	kJ/mol	Joback Method
hf	-661.12	kJ/mol	Joback Method
hfus	29.14	kJ/mol	Joback Method
hvap	69.18	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.992		Crippen Method
mcvol	242.670	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	814.75	K	Joback Method
tc	1056.67	K	Joback Method
tf	609.88	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.44	J/molxK	814.75	Joback Method
cpg	855.36	J/molxK	855.07	Joback Method
cpg	880.74	J/molxK	895.39	Joback Method
cpg	906.97	J/molxK	935.71	Joback Method
cpg	934.46	J/molxK	976.03	Joback Method
cpg	963.61	J/molxK	1016.35	Joback Method
cpg	994.84	J/molxK	1056.67	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=B6005242&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

Latest version available from:

<https://www.chemeo.com/cid/116-099-4/4-6-Ethano-1h-8h-pyrano-3-4-c-pyran-1-8-dione-hexahydro-3-3-6-trimethyl-8>

Generated by Cheméo on 2024-05-08 06:49:36.429297707 +0000 UTC m=+17440225.349875029.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.