5-Acetonyl-5-propyl-hexahydropyrimidin-2,4,6-tric

Other names: Dipropylbarbituric acid M (oxo)
Inchi: InChI=1S/C10H14N2O4/c1-3-4-10(5-6(2)13)7(14)11-9(16)12-8(10)15/h3-5H2,1-2H3,(H2
InchiKey: IPOXMTBHRJWWSO-UHFFFAOYSA-N
Formula: C10H14N2O4
SMILES: CCCC1(CC(C)=O)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 226.23

Physical Properties

Property code	Value	Unit	Source
gf	-268.99	kJ/mol	Joback Method
hf	-630.23	kJ/mol	Joback Method
hfus	26.50	kJ/mol	Joback Method
hvap	70.13	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.118		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	802.42	K	Joback Method
tc	1059.76	K	Joback Method
tf	698.39	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.34	J/mol×K	802.42	Joback Method
cpg	525.62	J/mol×K	845.31	Joback Method
cpg	540.96	J/mol×K	888.20	Joback Method
cpg	555.35	J/mol×K	931.09	Joback Method
cpg	568.80	J/mol×K	973.98	Joback Method
cpg	581.30	J/mol×K	1016.87	Joback Method
cpg	592.85	J/mol×K	1059.76	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=U281578&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume