Dipropylbarbituric acid M (OH), #1

Inchi: InChI=1S/C10H16N2O4/c1-3-5-10(6(13)4-2)7(14)11-9(16)12-8(10)15/h6,13H,3-5H2,1-2H
InchiKey: ATZJSQLJMQYLJI-UHFFFAOYSA-N
Formula: C10H16N2O4
SMILES: CCCC1(C(O)CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 228.25

Physical Properties

Property code	Value	Unit	Source
gf	-279.33	kJ/mol	Joback Method
hf	-675.16	kJ/mol	Joback Method
hfus	25.47	kJ/mol	Joback Method
hvap	79.68	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	-0.090		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	840.29	K	Joback Method
tc	1077.22	K	Joback Method
tf	694.28	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.03	J/mol×K	840.29	Joback Method
cpg	566.02	J/mol×K	879.78	Joback Method
cpg	580.20	J/mol×K	919.27	Joback Method
cpg	593.57	J/mol×K	958.75	Joback Method
cpg	606.14	J/mol×K	998.24	Joback Method
cpg	617.92	J/mol×K	1037.73	Joback Method
cpg	628.91	J/mol×K	1077.22	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=R57416&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