Butalbital M (OH)

Inchi: InChI=1S/C10H16N2O4/c1-4-9(3,16)10(5-2)6(13)11-8(15)12-7(10)14/h16H,4-5H2,1-3H3
InchiKey: POJYMHZIXHUWHN-UHFFFAOYSA-N
Formula: C10H16N2O4
SMILES: CCC(C)(O)C1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 228.25

Physical Properties

Property code	Value	Unit	Source
gf	-274.05	kJ/mol	Joback Method
hf	-678.63	kJ/mol	Joback Method
hfus	21.58	kJ/mol	Joback Method
hvap	78.77	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	-0.090		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	837.50	K	Joback Method
tc	1081.64	K	Joback Method
tf	711.70	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.85	J/mol×K	837.50	Joback Method
cpg	566.96	J/mol×K	878.19	Joback Method
cpg	581.28	J/mol×K	918.88	Joback Method
cpg	594.85	J/mol×K	959.57	Joback Method
cpg	607.69	J/mol×K	1000.26	Joback Method
cpg	619.86	J/mol×K	1040.95	Joback Method
cpg	631.37	J/mol×K	1081.64	Joback Method

Sources

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=R57331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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