Butylone M (dihydro), 2Ac

Inchi: InChI=1S/C16H21NO5/c1-5-13(17(4)10(2)18)16(22-11(3)19)12-6-7-14-15(8-12)21-9-20-
InchiKey: UNKMPYKKMAKTIC-UHFFFAOYSA-N
Formula: C16H21NO5
SMILES: CCC(C(OC(C)=O)c1ccc2c(c1)OCO2)N(C)C(C)=O
Mol. weight [g/mol]: 307.34

Physical Properties

Property code	Value	Unit	Source
gf	-183.73	kJ/mol	Joback Method
hf	-631.25	kJ/mol	Joback Method
hfus	43.84	kJ/mol	Joback Method
hvap	81.22	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.276		Crippen Method
mcvol	232.410	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	809.15	K	Joback Method
tc	1025.91	K	Joback Method
tf	521.42	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.76	J/mol×K	809.15	Joback Method
cpg	717.89	J/mol×K	845.28	Joback Method
cpg	731.03	J/mol×K	881.40	Joback Method
cpg	743.24	J/mol×K	917.53	Joback Method
cpg	754.57	J/mol×K	953.65	Joback Method
cpg	765.10	J/mol×K	989.78	Joback Method
cpg	774.89	J/mol×K	1025.91	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=R615797&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