Butylone M (demethylenyl, 3-O-methyl), 2Ac

Inchi: InChI=1S/C16H21NO5/c1-6-13(17(4)10(2)18)16(20)12-7-8-14(22-11(3)19)15(9-12)21-5/l
InchiKey: OSIBURBXMQMLCX-UHFFFAOYSA-N
Formula: C16H21NO5
SMILES: CCC(C(=O)c1ccc(OC(C)=O)c(OC)c1)N(C)C(C)=O
Mol. weight [g/mol]: 307.34

Physical Properties

Property code	Value	Unit	Source
gf	-311.43	kJ/mol	Joback Method
hf	-699.91	kJ/mol	Joback Method
hfus	37.13	kJ/mol	Joback Method
hvap	81.52	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.060		Crippen Method
mcvol	238.970	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	820.57	K	Joback Method
tc	1031.04	K	Joback Method
tf	533.26	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.62	J/mol×K	820.57	Joback Method
cpg	718.19	J/mol×K	855.65	Joback Method
cpg	730.68	J/mol×K	890.73	Joback Method
cpg	742.10	J/mol×K	925.80	Joback Method
cpg	752.47	J/mol×K	960.88	Joback Method
cpg	761.79	J/mol×K	995.96	Joback Method
cpg	770.09	J/mol×K	1031.04	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=R615782&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