(S)-2-Butyl 2-deoxy-3,4,6-tri-O-methyl-2-(N-methylacetamido)

Inchi: InChI=1S/C16H31NO6/c1-8-10(2)22-16-13(17(4)11(3)18)15(21-7)14(20-6)12(23-16)9-19

InchiKey: XEIPZNANFWJBGB-LCIOIPORSA-N

Formula: C16H31NO6

SMILES: CCC(C)OC1OC(COC)C(OC)C(OC)C1N(C)C(C)=O

Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
gf	-449.25	kJ/mol	Joback Method
hf	-1111.82	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.050		Crippen Method
mcvol	266.340	ml/mol	McGowan Method
pc	1382.99	kPa	Joback Method
rinpol	1987.66		NIST Webbook
tb	748.85	K	Joback Method
tc	938.27	K	Joback Method
tf	443.39	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.07	J/mol×K	748.85	Joback Method
cpg	873.29	J/mol×K	780.42	Joback Method
cpg	892.25	J/mol×K	811.99	Joback Method
cpg	909.91	J/mol×K	843.56	Joback Method
cpg	926.26	J/mol×K	875.13	Joback Method
cpg	941.27	J/mol×K	906.70	Joback Method
cpg	954.93	J/mol×K	938.27	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=R391609&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