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

Inchi: InChI=1S/C18H33NO6/c1-12(20)19(2)15-17(23-5)16(22-4)14(11-21-3)25-18(15)24-13-9-

InchiKey: VHHBUELNGTZTNP-KFGODFMUSA-N

Formula: C18H33NO6

SMILES: COCC1OC(OC2CCCCC2)C(N(C)C(C)=O)C(OC)C1OC

Mol. weight [g/mol]: 359.46

Physical Properties

Property code	Value	Unit	Source
gf	-405.52	kJ/mol	Joback Method
hf	-1093.50	kJ/mol	Joback Method
hfus	47.68	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.584		Crippen Method
mcvol	283.660	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
rinpol	2419.86		NIST Webbook
rinpol	2419.86		NIST Webbook
tb	814.60	K	Joback Method
tc	1021.11	K	Joback Method
tf	488.31	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.91	J/mol×K	814.60	Joback Method
cpg	993.27	J/mol×K	849.02	Joback Method
cpg	1012.81	J/mol×K	883.44	Joback Method
cpg	1030.53	J/mol×K	917.85	Joback Method
cpg	1046.41	J/mol×K	952.27	Joback Method
cpg	1060.41	J/mol×K	986.69	Joback Method
cpg	1072.52	J/mol×K	1021.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496289&Units=SI
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

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

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