N-Methyl 2-deoxy-3 4,6-tri-O-methyl-2-(N-ethylacetamido) -«beta» - D- galactopyranoside

InchI: InChI=1S/C13H25NO6/c1-8(15)14(2)10-12(18-5)11(17-4)9(7-16-3)20-13(10)19-6/h9-13H
InchiKey: LLDFFWSIFJDSHK-WJTVCTBASA-N
Formula: C13H25NO6
SMILES: COCC1OC(OC)C(N(C)C(C)=O)C(OC)C1OC
Mol. weight [g/mol]: 291.34

Physical Properties

Property code	Value	Unit	Source
gf	-472.07	kJ/mol	Joback Method
hf	-1044.62	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	5.01e-03		Crippen Method
logp	-0.119		Crippen Method
mcvol	224.070	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1876.72		NIST Webbook
tb	680.65	K	Joback Method
tc	870.20	K	Joback Method
tf	424.58	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.56	J/mol×K	680.65	Joback Method
cpg	696.96	J/mol×K	712.24	Joback Method
cpg	715.33	J/mol×K	743.83	Joback Method
cpg	732.64	J/mol×K	775.43	Joback Method
cpg	748.85	J/mol×K	807.02	Joback Method
cpg	763.93	J/mol×K	838.61	Joback Method
cpg	777.86	J/mol×K	870.20	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=R391570&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