

Galactopyranoside, p-nitrophenyl, tetraacetate, beta-d-

Inchi:	InChI=1S/C20H23NO12/c1-10(22)28-9-16-17(29-11(2)23)18(30-12(3)24)19(31-13(4)25)
InchiKey:	BEUISCKWILNFIL-LCWAXJCOSA-N
Formula:	C20H23NO12
SMILES:	CC(=O)OCC1OC(Oc2ccc([N+](=O)[O-])cc2)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	469.40
CAS:	2872-66-4

Physical Properties

Property code	Value	Unit	Source
gf	-877.34	kJ/mol	Joback Method
hf	-1512.29	kJ/mol	Joback Method
hfus	69.00	kJ/mol	Joback Method
hvap	122.38	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	1.057		Crippen Method
mcvol	316.960	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
tb	1195.90	K	Joback Method
tc	1464.16	K	Joback Method
tf	825.57	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.74	J/molxK	1195.90	Joback Method
cpg	1071.62	J/molxK	1240.61	Joback Method
cpg	1062.62	J/molxK	1285.32	Joback Method
cpg	1049.63	J/molxK	1330.03	Joback Method
cpg	1032.56	J/molxK	1374.74	Joback Method
cpg	1011.32	J/molxK	1419.45	Joback Method
cpg	985.82	J/molxK	1464.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2872664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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