

1,2:5,6-Dianhydrogalactitol

Other names:	Dianhydrodulcitol Dianhydrogalactitol Dulcitol diepoxide DAD DAG Galactitol, 1,2:5,6-dianhydro- NSC 132313 1,2:5,6-Dianhydrodulcitol 1,2:5,6-Diepoxydulcitol 1,2-5,6-Dianhydro-dulcitol
Inchi:	InChI=1S/C6H10O4/c7-5(3-1-9-3)6(8)4-2-10-4/h3-8H,1-2H2
InchiKey:	AAFJXZWCNVJTMK-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	OC(C1CO1)C(O)C1CO1
Mol. weight [g/mol]:	146.14
CAS:	23261-20-3

Physical Properties

Property code	Value	Unit	Source
gf	-329.62	kJ/mol	Joback Method
hf	-600.59	kJ/mol	Joback Method
h _{fus}	24.65	kJ/mol	Joback Method
h _{vap}	70.38	kJ/mol	Joback Method
log ₁₀ ws	0.73		Crippen Method
logp	-1.494		Crippen Method
m _{cvol}	97.160	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
tb	587.54	K	Joback Method
tc	772.67	K	Joback Method
tf	338.04	K	Joback Method
vc	0.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.27	J/mol×K	587.54	Joback Method
cpg	288.20	J/mol×K	618.40	Joback Method
cpg	296.56	J/mol×K	649.25	Joback Method
cpg	304.40	J/mol×K	680.11	Joback Method
cpg	311.76	J/mol×K	710.96	Joback Method
cpg	318.68	J/mol×K	741.82	Joback Method
cpg	325.21	J/mol×K	772.67	Joback Method
dvisc	0.0252275	Paxs	338.04	Joback Method
dvisc	0.0073346	Paxs	379.62	Joback Method
dvisc	0.0027215	Paxs	421.21	Joback Method
dvisc	0.0012068	Paxs	462.79	Joback Method
dvisc	0.0006119	Paxs	504.37	Joback Method
dvisc	0.0003441	Paxs	545.96	Joback Method
dvisc	0.0002099	Paxs	587.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23261203&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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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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