Quercitol

Other names: d-quercitol
Inchi: InChI=1S/C6H12O5/c7-2-1-3(8)5(10)6(11)4(2)9/h2-11H,1H2
InchiKey: IMPKVMRTXBRHRB-UHFFFAOYSA-N
Formula: C6H12O5
SMILES: OC1CC(O)C(O)C(O)C1O
Mol. weight [g/mol]: 164.16
CAS: 488-73-3

Physical Properties

Property code	Value	Unit	Source
gf	-690.85	kJ/mol	Joback Method
hf	-955.36	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	111.54	kJ/mol	Joback Method
log10ws	-0.17		Aqueous Solubility Prediction Method
logp	-2.805		Crippen Method
mcvol	113.890	ml/mol	McGowan Method
pc	6288.83	kPa	Joback Method
rinpol	1834.00		NIST Webbook
tb	798.45	K	Joback Method
tc	979.54	K	Joback Method
tf	451.90	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.65	J/mol×K	798.45	Joback Method
cpg	399.53	J/mol×K	828.63	Joback Method
cpg	406.86	J/mol×K	858.81	Joback Method
cpg	413.65	J/mol×K	889.00	Joback Method
cpg	419.89	J/mol×K	919.18	Joback Method
cpg	425.59	J/mol×K	949.36	Joback Method

cpg	430.75	J/mol×K	979.54	Joback Method
dvisc	0.0010248	Pa×s	451.90	Joback Method
dvisc	0.0001184	Pa×s	509.66	Joback Method
dvisc	0.0000212	Pa×s	567.42	Joback Method
dvisc	0.0000052	Pa×s	625.17	Joback Method
dvisc	0.0000016	Pa×s	682.93	Joback Method
dvisc	0.0000006	Pa×s	740.69	Joback Method
dvisc	0.0000003	Pa×s	798.45	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C488733&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
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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