2,5-Dimethylbenzene-1,3-diol

Other names: 1,3-Dihydroxy-2,5-dimethylbenzene
Inchi: InChI=1S/C8H10O2/c1-5-3-7(9)6(2)8(10)4-5/h3-4,9-10H,1-2H3
InchiKey: GHVHDYYKJYXFGU-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: Cc1cc(O)c(C)c(O)c1
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
af	0.6218		Cheméo Relay (1.0)
gf	-189.98	kJ/mol	Joback Method
hf	-321.95	kJ/mol	Cheméo Relay (1.0)
hfus	21.69	kJ/mol	Joback Method
hvap	76.81	kJ/mol	Cheméo Relay (1.0)
ie	8.13	eV	Cheméo Relay (1.0)
log10ws	-1.55		Cheméo Relay (1.0)
logp	1.715		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	5312.41	kPa	Joback Method
rinpol	1429.70		NIST Webbook
rinpol	1429.70		NIST Webbook
tb	542.99	K	Cheméo Relay (1.0)
tc	755.24	K	Cheméo Relay (1.0)
tf	403.58	K	Cheméo Relay (1.0)
vc	0.387	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.26	J/mol×K	774.89	Joback Method
cpg	319.75	J/mol×K	814.79	Joback Method
cpg	278.66	J/mol×K	615.25	Joback Method
cpg	287.88	J/mol×K	655.16	Joback Method
cpg	296.46	J/mol×K	695.07	Joback Method

cpg	304.55	J/mol×K	734.98	Joback Method
cpg	268.68	J/mol×K	575.34	Joback Method
dvisc	0.0000664	Pa×s	486.65	Joback Method
dvisc	0.0001205	Pa×s	464.47	Joback Method
dvisc	0.0002320	Pa×s	442.30	Joback Method
dvisc	0.0000386	Pa×s	508.82	Joback Method
dvisc	0.0000234	Pa×s	530.99	Joback Method
dvisc	0.0000148	Pa×s	553.17	Joback Method
dvisc	0.0000097	Pa×s	575.34	Joback Method
hvapt	74.70	kJ/mol	426.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C488879&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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