O-XYLENE-ALPHA,ALPHA'-DIOL

Other names: 2-Hydroxymethylbenzenemethanol
o-xylene-«alpha»,«alpha»'-diol
Inchi: InChI=1S/C8H10O2/c9-5-7-3-1-2-4-8(7)6-10/h1-4,9-10H,5-6H2
InchiKey: XMUZQOKACOLCSS-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: OCc1ccccc1CO
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
af	0.7257		Cheméo Relay (1.0)
hf	-259.87	kJ/mol	Cheméo Relay (1.0)
hfus	18.30	kJ/mol	Joback Method
hvap	96.26	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-1.05		Cheméo Relay (1.0)
logp	0.671		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	538.35	K	Cheméo Relay (1.0)
tc	795.42	K	Cheméo Relay (1.0)
tf	339.40 ± 3.00	K	NIST Webbook
vc	0.395	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.61	J/mol×K	598.46	Joback Method
cpg	276.22	J/mol×K	629.69	Joback Method
cpg	284.35	J/mol×K	660.93	Joback Method
cpg	292.04	J/mol×K	692.16	Joback Method
cpg	299.29	J/mol×K	723.39	Joback Method
cpg	306.14	J/mol×K	754.63	Joback Method
cpg	312.59	J/mol×K	785.86	Joback Method

dvisc	0.0100764	Pa×s	340.50	Joback Method
dvisc	0.0023013	Pa×s	383.49	Joback Method
dvisc	0.0007079	Pa×s	426.49	Joback Method
dvisc	0.0002702	Pa×s	469.48	Joback Method
dvisc	0.0001212	Pa×s	512.47	Joback Method
dvisc	0.0000616	Pa×s	555.47	Joback Method
dvisc	0.0000345	Pa×s	598.46	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C612146&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume