2,7-Dimethyl-2,7-octanediol

Other names: 2,7-Octanediol, 2,7-dimethyl-
Inchi: InChI=1S/C10H22O2/c1-9(2,11)7-5-6-8-10(3,4)12/h11-12H,5-8H2,1-4H3
InchiKey: LZMSJLJRUYKOQD-UHFFFAOYSA-N
Formula: C10H22O2
SMILES: CC(C)(O)CCCCC(C)(C)O
Mol. weight [g/mol]: 174.28
CAS: 19781-07-8

Physical Properties

Property code	Value	Unit	Source
chs	-6349.00 ± 2.00	kJ/mol	NIST Webbook
gf	-234.64	kJ/mol	Joback Method
hf	-571.69	kJ/mol	Joback Method
hfs	-730.00 ± 2.00	kJ/mol	NIST Webbook
hfus	15.00	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.089		Crippen Method
mcvol	163.500	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
tb	606.10	K	Joback Method
tc	775.93	K	Joback Method
tf	328.94	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.02	J/mol×K	606.10	Joback Method
cpg	504.05	J/mol×K	747.63	Joback Method
cpg	494.01	J/mol×K	719.32	Joback Method
cpg	483.42	J/mol×K	691.02	Joback Method
cpg	472.25	J/mol×K	662.71	Joback Method
cpg	460.46	J/mol×K	634.41	Joback Method

cpg	513.59	J/mol×K	775.93	Joback Method
dvisc	0.0000230	Pa×s	606.10	Joback Method
dvisc	0.0000465	Pa×s	559.91	Joback Method
dvisc	0.0001068	Pa×s	513.71	Joback Method
dvisc	0.0002887	Pa×s	467.52	Joback Method
dvisc	0.0009711	Pa×s	421.33	Joback Method
dvisc	0.0044032	Pa×s	375.13	Joback Method
dvisc	0.0305262	Pa×s	328.94	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume