

2,6-dimethyloct-7-ene-2,3,6-triol

Inchi:	InChI=1S/C10H20O3/c1-5-10(4,13)7-6-8(11)9(2,3)12/h5,8,11-13H,1,6-7H2,2-4H3
InchiKey:	CNYFGLAROLNGDG-UHFFFAOYSA-N
Formula:	C10H20O3
SMILES:	C=CC(C)(O)CCC(O)C(C)(C)O
Mol. weight [g/mol]:	188.26

Physical Properties

Property code	Value	Unit	Source
gf	-286.06	kJ/mol	Joback Method
hf	-603.77	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	84.24	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	0.835		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
ripol	2425.00		NIST Webbook
tb	694.52	K	Joback Method
tc	867.17	K	Joback Method
tf	373.00	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.87	J/molxK	694.52	Joback Method
cpg	526.33	J/molxK	838.39	Joback Method
cpg	518.18	J/molxK	809.62	Joback Method
cpg	509.60	J/molxK	780.84	Joback Method
cpg	500.55	J/molxK	752.07	Joback Method
cpg	490.99	J/molxK	723.29	Joback Method
cpg	534.10	J/molxK	867.17	Joback Method
dvisc	0.0000028	Paxs	694.52	Joback Method
dvisc	0.0000064	Paxs	640.93	Joback Method

dvisc	0.0000170	Paxs	587.35	Joback Method
dvisc	0.0000549	Paxs	533.76	Joback Method
dvisc	0.0002308	Paxs	480.17	Joback Method
dvisc	0.0013902	Paxs	426.59	Joback Method
dvisc	0.0140305	Paxs	373.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R297884&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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