1,2-Propanediol diformate

Inchi: InChI=1S/C5H8O4/c1-5(9-4-7)2-8-3-6/h3-5H,2H2,1H3
InchiKey: DUYOHDPGXMPOKD-UHFFFAOYSA-N
Formula: C5H8O4
SMILES: CC(COC=O)OC=O
Mol. weight [g/mol]: 132.11
CAS: 53818-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-420.26	kJ/mol	Joback Method
hf	-587.41	kJ/mol	Joback Method
hfus	12.14	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
log10ws	0.25		Crippen Method
logp	-0.279		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	455.52	K	Joback Method
tc	639.75	K	Joback Method
tf	259.57	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.02	J/mol×K	455.52	Joback Method
cpg	208.66	J/mol×K	486.23	Joback Method
cpg	216.09	J/mol×K	516.93	Joback Method
cpg	223.30	J/mol×K	547.64	Joback Method
cpg	230.28	J/mol×K	578.34	Joback Method
cpg	237.01	J/mol×K	609.05	Joback Method
cpg	243.49	J/mol×K	639.75	Joback Method
dvisc	0.0034584	Pa×s	259.57	Joback Method
dvisc	0.0018537	Pa×s	292.23	Joback Method

dvisc	0.0011263	Pa×s	324.89	Joback Method
dvisc	0.0007495	Pa×s	357.54	Joback Method
dvisc	0.0005340	Pa×s	390.20	Joback Method
dvisc	0.0004009	Pa×s	422.86	Joback Method
dvisc	0.0003136	Pa×s	455.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.50 ± 0.50	K	2.00	NIST Webbook

Sources

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=C53818147&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume