1,3,5-Pentanetricarboxylic acid, 3-hydroxy-2-methyl, trimethyl ester

Inchi: InChI=1S/C11H18O7/c1-16-8(12)4-6-11(15,10(14)18-3)7-5-9(13)17-2/h15H,4-7H2,1-3H3

InchiKey: XUAJBOMRONHLNB-UHFFFAOYSA-N

Formula: C11H18O7

SMILES: COC(=O)CCC(O)(CCC(=O)OC)C(=O)OC

Mol. weight [g/mol]: 262.26

Physical Properties

Property code	Value	Unit	Source
gf	-794.00	kJ/mol	Joback Method
hf	-1165.75	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	82.93	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	-0.203		Crippen Method
mcvol	194.040	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1473.00		NIST Webbook
tb	768.90	K	Joback Method
tc	958.07	K	Joback Method
tf	493.45	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.53	J/mol×K	768.90	Joback Method
cpg	577.41	J/mol×K	800.43	Joback Method
cpg	587.56	J/mol×K	831.96	Joback Method
cpg	596.98	J/mol×K	863.49	Joback Method
cpg	605.69	J/mol×K	895.01	Joback Method
cpg	613.68	J/mol×K	926.54	Joback Method
cpg	620.96	J/mol×K	958.07	Joback Method
dvisc	0.0004983	Pa×s	493.45	Joback Method
dvisc	0.0002328	Pa×s	539.36	Joback Method

dvisc	0.0001226	Pa×s	585.27	Joback Method
dvisc	0.0000709	Pa×s	631.17	Joback Method
dvisc	0.0000441	Pa×s	677.08	Joback Method
dvisc	0.0000292	Pa×s	722.99	Joback Method
dvisc	0.0000203	Pa×s	768.90	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R106382&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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