

1,3,5-tris-(Hydroxymethyl)benzene triacetate

Inchi:	InChI=1S/C15H18O6/c1-10(16)19-7-13-4-14(8-20-11(2)17)6-15(5-13)9-21-12(3)18/h4-6H
InchiKey:	JTUPDNAWXLSTQJ-UHFFFAOYSA-N
Formula:	C15H18O6
SMILES:	CC(=O)OCc1cc(COC(C)=O)cc(COC(C)=O)c1
Mol. weight [g/mol]:	294.30

Physical Properties

Property code	Value	Unit	Source
gf	-533.19	kJ/mol	Joback Method
hf	-873.74	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	1.876		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinsol	2010.00		NIST Webbook
tb	808.11	K	Joback Method
tc	1018.00	K	Joback Method
tf	526.75	K	Joback Method
vc	0.840	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.51	J/molxK	808.11	Joback Method
cpg	647.19	J/molxK	843.09	Joback Method
cpg	658.83	J/molxK	878.07	Joback Method
cpg	669.43	J/molxK	913.05	Joback Method
cpg	678.96	J/molxK	948.03	Joback Method
cpg	687.42	J/molxK	983.02	Joback Method
cpg	694.80	J/molxK	1018.00	Joback Method
dvisc	0.0004943	Paxs	526.75	Joback Method
dvisc	0.0003221	Paxs	573.64	Joback Method

dvisc	0.0002240	Paxs	620.54	Joback Method
dvisc	0.0001639	Paxs	667.43	Joback Method
dvisc	0.0001250	Paxs	714.32	Joback Method
dvisc	0.0000985	Paxs	761.22	Joback Method
dvisc	0.0000798	Paxs	808.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R96347&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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