

Torquatone

Inchi:	InChI=1S/C16H24O4/c1-9(2)8-12(17)13-15(19-6)10(3)14(18-5)11(4)16(13)20-7/h9H,8H2
InchiKey:	PYUCCSKQLHUKCA-UHFFFAOYSA-N
Formula:	C16H24O4
SMILES:	COc1c(C)c(OC)c(C(=O)CC(C)C)c(OC)c1C
Mol. weight [g/mol]:	280.36
CAS:	3567-96-2

Physical Properties

Property code	Value	Unit	Source
gf	-298.26	kJ/mol	Joback Method
hf	-708.91	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	70.38	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.558		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2424.00		NIST Webbook
tb	737.75	K	Joback Method
tc	938.11	K	Joback Method
tf	460.72	K	Joback Method
vc	0.877	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.24	J/molxK	737.75	Joback Method
cpg	671.37	J/molxK	771.14	Joback Method
cpg	686.57	J/molxK	804.54	Joback Method
cpg	700.85	J/molxK	837.93	Joback Method
cpg	714.16	J/molxK	871.32	Joback Method
cpg	726.49	J/molxK	904.71	Joback Method
cpg	737.82	J/molxK	938.11	Joback Method
dvisc	0.0004199	Paxs	460.72	Joback Method
dvisc	0.0002694	Paxs	506.89	Joback Method
dvisc	0.0001862	Paxs	553.06	Joback Method
dvisc	0.0001362	Paxs	599.24	Joback Method
dvisc	0.0001042	Paxs	645.41	Joback Method
dvisc	0.0000826	Paxs	691.58	Joback Method
dvisc	0.0000674	Paxs	737.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3567962&Units=SI
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

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

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