

acetonylguaiacol

Inchi:	InChI=1S/C10H12O3/c1-8(11)7-13-10-6-4-3-5-9(10)12-2/h3-6H,7H2,1-2H3
InchiKey:	GBBBWTDKOLEAOC-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1ccccc1OCC(C)=O
Mol. weight [g/mol]:	180.20
CAS:	6437-46-3

Physical Properties

Property code	Value	Unit	Source
gf	-202.82	kJ/mol	Joback Method
hf	-401.69	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.663		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1541.10		NIST Webbook
rinpol	1541.10		NIST Webbook
tb	558.57	K	Joback Method
tc	770.06	K	Joback Method
tf	335.79	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.98	J/molxK	558.57	Joback Method
cpg	337.02	J/molxK	593.82	Joback Method
cpg	349.42	J/molxK	629.07	Joback Method
cpg	361.16	J/molxK	664.31	Joback Method
cpg	372.24	J/molxK	699.56	Joback Method
cpg	382.66	J/molxK	734.81	Joback Method
cpg	392.43	J/molxK	770.06	Joback Method

dvisc	0.0013400	Paxs	335.79	Joback Method
dvisc	0.0008036	Paxs	372.92	Joback Method
dvisc	0.0005287	Paxs	410.05	Joback Method
dvisc	0.0003728	Paxs	447.18	Joback Method
dvisc	0.0002774	Paxs	484.31	Joback Method
dvisc	0.0002153	Paxs	521.44	Joback Method
dvisc	0.0001728	Paxs	558.57	Joback Method

Sources

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=C6437463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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