

(E)-Azarone

Inchi:	InChI=1S/C12H16O3/c1-5-6-9-7-11(14-3)12(15-4)8-10(9)13-2/h5-8H,1-4H3/b6-5+
InchiKey:	RKFAZBXYICVSKP-AATRIKPKSA-N
Formula:	C12H16O3
SMILES:	CC=Cc1cc(OC)c(OC)cc1OC
Mol. weight [g/mol]:	208.25

Physical Properties

Property code	Value	Unit	Source
gf	-101.10	kJ/mol	Joback Method
hf	-368.33	kJ/mol	Joback Method
hfus	23.48	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.745		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1377.00		NIST Webbook
rinpol	1376.00		NIST Webbook
tb	587.00	K	Joback Method
tc	792.75	K	Joback Method
tf	350.59	K	Joback Method
vc	0.633	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.78	J/molxK	587.00	Joback Method
cpg	419.37	J/molxK	621.29	Joback Method
cpg	433.31	J/molxK	655.58	Joback Method
cpg	446.60	J/molxK	689.87	Joback Method
cpg	459.22	J/molxK	724.16	Joback Method
cpg	471.18	J/molxK	758.45	Joback Method
cpg	482.46	J/molxK	792.75	Joback Method
dvisc	0.0006142	Paxs	350.59	Joback Method

dvisc	0.0003804	Paxs	389.99	Joback Method
dvisc	0.0002572	Paxs	429.39	Joback Method
dvisc	0.0001858	Paxs	468.80	Joback Method
dvisc	0.0001411	Paxs	508.20	Joback Method
dvisc	0.0001115	Paxs	547.60	Joback Method
dvisc	0.0000910	Paxs	587.00	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=R615059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

Latest version available from:

<https://www.chemeo.com/cid/71-411-6/E-Azarone.pdf>

Generated by Cheméo on 2024-04-25 18:10:08.732758528 +0000 UTC m=+16357857.653335840.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.