

Yuzunone

Inchi:	InChI=1S/C11H16O/c1-3-5-6-7-8-9-10-11(12)4-2/h3,5-8H,1,4,9-10H2,2H3/b6-5+,8-7-
InchiKey:	AJRVUFGWENEBHO-MDAAKZFYSA-N
Formula:	C11H16O
SMILES:	C=CC=CC=CCCC(=O)CC
Mol. weight [g/mol]:	164.24

Physical Properties

Property code	Value	Unit	Source
gf	161.10	kJ/mol	Joback Method
hf	-23.08	kJ/mol	Joback Method
hfus	24.97	kJ/mol	Joback Method
hvap	46.07	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.044		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
ripol	1899.00		NIST Webbook
ripol	1899.00		NIST Webbook
tb	509.95	K	Joback Method
tc	700.42	K	Joback Method
tf	251.74	K	Joback Method
vc	0.599	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.11	J/molxK	509.95	Joback Method
cpg	349.11	J/molxK	541.70	Joback Method
cpg	362.32	J/molxK	573.44	Joback Method
cpg	374.81	J/molxK	605.19	Joback Method
cpg	386.61	J/molxK	636.93	Joback Method
cpg	397.76	J/molxK	668.68	Joback Method
cpg	408.31	J/molxK	700.42	Joback Method
dvisc	0.0035611	Paxs	251.74	Joback Method

dvisc	0.0015097	Paxs	294.78	Joback Method
dvisc	0.0007965	Paxs	337.81	Joback Method
dvisc	0.0004855	Paxs	380.85	Joback Method
dvisc	0.0003273	Paxs	423.88	Joback Method
dvisc	0.0002372	Paxs	466.92	Joback Method
dvisc	0.0001816	Paxs	509.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R616067&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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