

Yuzuol

Inchi: InChI=1S/C11H18O/c1-3-5-6-7-8-10-11(12)9-4-2/h3,5-8,11-12H,1,4,9-10H2,2H3/b6-5+,8-7-
InchiKey: YAWVREQAXOUSRY-MDAAKZFYSA-N
Formula: C11H18O
SMILES: C=CC=CC=CCC(O)CCC
Mol. weight [g/mol]: 166.26

Physical Properties

Property code	Value	Unit	Source
gf	150.76	kJ/mol	Joback Method
hf	-68.01	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Joback Method
hvap	55.62	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.836		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
ripol	1986.00		NIST Webbook
tb	547.82	K	Joback Method
tc	724.07	K	Joback Method
tf	247.63	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.48	J/mol×K	547.82	Joback Method
cpg	385.38	J/mol×K	577.19	Joback Method
cpg	397.63	J/mol×K	606.57	Joback Method
cpg	409.25	J/mol×K	635.94	Joback Method
cpg	420.29	J/mol×K	665.32	Joback Method
cpg	430.78	J/mol×K	694.69	Joback Method
cpg	440.76	J/mol×K	724.07	Joback Method
dvisc	0.0525915	Pa×s	247.63	Joback Method
dvisc	0.0069062	Pa×s	297.66	Joback Method

dvisc	0.0016267	Pa×s	347.69	Joback Method
dvisc	0.0005512	Pa×s	397.73	Joback Method
dvisc	0.0002379	Pa×s	447.76	Joback Method
dvisc	0.0001216	Pa×s	497.79	Joback Method
dvisc	0.0000702	Pa×s	547.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R616072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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