

2-decanon-3-ol

Inchi:	InChI=1S/C10H20O2/c1-3-4-5-6-7-8-10(12)9(2)11/h10,12H,3-8H2,1-2H3
InchiKey:	WQMUDPTXGSGWFD-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCCC(O)C(C)=O
Mol. weight [g/mol]:	172.26

Physical Properties

Property code	Value	Unit	Source
gf	-234.86	kJ/mol	Joback Method
hf	-519.82	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.297		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
ripol	1889.00		NIST Webbook
ripol	1889.00		NIST Webbook
tb	573.81	K	Joback Method
tc	743.57	K	Joback Method
tf	298.21	K	Joback Method
vc	0.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.15	J/molxK	573.81	Joback Method
cpg	415.84	J/molxK	602.10	Joback Method
cpg	427.99	J/molxK	630.40	Joback Method
cpg	439.61	J/molxK	658.69	Joback Method
cpg	450.71	J/molxK	686.99	Joback Method
cpg	461.31	J/molxK	715.28	Joback Method
cpg	471.43	J/molxK	743.57	Joback Method
dvisc	0.0185428	Paxs	298.21	Joback Method

dvisc	0.0043186	Paxs	344.14	Joback Method
dvisc	0.0014176	Paxs	390.08	Joback Method
dvisc	0.0005884	Paxs	436.01	Joback Method
dvisc	0.0002888	Paxs	481.94	Joback Method
dvisc	0.0001605	Paxs	527.88	Joback Method
dvisc	0.0000979	Paxs	573.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R240863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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