

Hydratropic acid, isopropyl ester

Inchi:	InChI=1S/C12H16O2/c1-9(2)14-12(13)10(3)11-7-5-4-6-8-11/h4-10H,1-3H3
InchiKey:	PLBPZACPOTWOJD-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(C)OC(=O)C(C)c1ccccc1
Mol. weight [g/mol]:	192.25

Physical Properties

Property code	Value	Unit	Source
gf	-76.23	kJ/mol	Joback Method
hf	-309.84	kJ/mol	Joback Method
hfus	16.62	kJ/mol	Joback Method
hvap	52.96	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.742		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1763.00		NIST Webbook
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tb	576.05	K	Joback Method
tc	790.82	K	Joback Method
tf	293.58	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.78	J/mol×K	576.05	Joback Method
cpg	465.34	J/mol×K	755.03	Joback Method
cpg	453.01	J/mol×K	719.23	Joback Method
cpg	439.81	J/mol×K	683.44	Joback Method
cpg	425.72	J/mol×K	647.64	Joback Method
cpg	410.72	J/mol×K	611.85	Joback Method
cpg	476.83	J/mol×K	790.82	Joback Method
dvisc	0.0001615	Pa×s	576.05	Joback Method

dvisc	0.0002172	Pa×s	528.97	Joback Method
dvisc	0.0003095	Pa×s	481.89	Joback Method
dvisc	0.0004761	Pa×s	434.81	Joback Method
dvisc	0.0008134	Pa×s	387.74	Joback Method
dvisc	0.0016112	Pa×s	340.66	Joback Method
dvisc	0.0039738	Pa×s	293.58	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415059&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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