

Alpha-cyclopropyl-alpha,p-dimethylbenzyl alcohol

Other names:	«alpha»-cyclopropyl-«alpha»-4-dimethylbenzyl alcohol
Inchi:	InChI=1S/C12H16O/c1-9-3-5-10(6-4-9)12(2,13)11-7-8-11/h3-6,11,13H,7-8H2,1-2H3
InchiKey:	IJYCFWNBUFSFNP-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	<chem>Cc1ccc(C(C)(O)C2CC2)cc1</chem>
Mol. weight [g/mol]:	176.25
CAS:	33446-27-4

Physical Properties

Property code	Value	Unit	Source
gf	79.71	kJ/mol	Joback Method
hf	-154.13	kJ/mol	Joback Method
hfus	15.30	kJ/mol	Joback Method
hvap	60.54	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.613		Crippen Method
mcvol	151.190	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
tb	601.31	K	Joback Method
tc	814.27	K	Joback Method
tf	345.12	K	Joback Method
vc	0.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.25	J/mol×K	601.31	Joback Method
cpg	410.12	J/mol×K	636.80	Joback Method
cpg	423.94	J/mol×K	672.30	Joback Method
cpg	436.79	J/mol×K	707.79	Joback Method
cpg	448.76	J/mol×K	743.29	Joback Method
cpg	459.93	J/mol×K	778.78	Joback Method
cpg	470.39	J/mol×K	814.27	Joback Method
dvisc	0.0052985	Paxs	345.12	Joback Method

dvisc	0.0021231	Paxs	387.82	Joback Method
dvisc	0.0010199	Paxs	430.52	Joback Method
dvisc	0.0005593	Paxs	473.21	Joback Method
dvisc	0.0003387	Paxs	515.91	Joback Method
dvisc	0.0002215	Paxs	558.61	Joback Method
dvisc	0.0001539	Paxs	601.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33446274&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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