

3-isopropenyl-2,2-dimethylcyclobutane-methanol

Inchi:	InChI=1S/C10H18O/c1-7(2)9-5-8(6-11)10(9,3)4/h8-9,11H,1,5-6H2,2-4H3
InchiKey:	PESUSZICVBPIGK-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=C(C)C1CC(CO)C1(C)C
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
gf	3.53	kJ/mol	Joback Method
hf	-245.12	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.217		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1152.00		NIST Webbook
rinpol	1150.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1601.00		NIST Webbook
tb	518.85	K	Joback Method
tc	705.69	K	Joback Method
tf	277.40	K	Joback Method
vc	0.541	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.52	J/molxK	518.85	Joback Method
cpg	364.46	J/molxK	549.99	Joback Method
cpg	378.56	J/molxK	581.13	Joback Method
cpg	391.90	J/molxK	612.27	Joback Method
cpg	404.56	J/molxK	643.41	Joback Method
cpg	416.63	J/molxK	674.55	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=R504424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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