

1,4-Dimethyl-2-(2-methylpropyl)-(1 «alpha»,2 «beta

Inchi:	InChI=1S/C12H24/c1-9(2)7-12-8-10(3)5-6-11(12)4/h9-12H,5-8H2,1-4H3/t10-,11+,12+/m0
InchiKey:	ZYJPKZNMPTYTPA-QJPTWQEYSA-N
Formula:	C12H24
SMILES:	CC(C)CC1CC(C)CCC1C
Mol. weight [g/mol]:	168.32

Physical Properties

Property code	Value	Unit	Source
gf	56.75	kJ/mol	Joback Method
hf	-282.65	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	41.73	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	4.105		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	189.20		NIST Webbook
tb	483.73	K	Joback Method
tc	679.68	K	Joback Method
tf	208.90	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.76	J/molxK	483.73	Joback Method
cpg	416.96	J/molxK	516.39	Joback Method
cpg	438.15	J/molxK	549.05	Joback Method
cpg	458.35	J/molxK	581.71	Joback Method
cpg	477.58	J/molxK	614.36	Joback Method
cpg	495.86	J/molxK	647.02	Joback Method
cpg	513.20	J/molxK	679.68	Joback Method
dvisc	0.0049638	Paxs	208.90	Joback Method
dvisc	0.0019139	Paxs	254.71	Joback Method

dvisc	0.0009867	Paxs	300.51	Joback Method
dvisc	0.0006061	Paxs	346.32	Joback Method
dvisc	0.0004173	Paxs	392.12	Joback Method
dvisc	0.0003106	Paxs	437.93	Joback Method
dvisc	0.0002445	Paxs	483.73	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=R516586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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