

2,4-dimethyl-2,3-isopropyl-pentane

Inchi: InChI=1S/C13H28/c1-9(2)12(10(3)4)13(7,8)11(5)6/h9-12H,1-8H3
InchiKey: KKCMURFTKJKCG-UHFFFAOYSA-N
Formula: C13H28
SMILES: CC(C)C(C(C)C)C(C)(C)C(C)C
Mol. weight [g/mol]: 184.36

Physical Properties

Property code	Value	Unit	Source
gf	51.66	kJ/mol	Joback Method
hf	-341.52	kJ/mol	Joback Method
hfus	7.92	kJ/mol	Joback Method
hvap	41.68	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	4.597		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	928.00		NIST Webbook
tb	491.85	K	Joback Method
tc	675.28	K	Joback Method
tf	178.69	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.14	J/mol×K	491.85	Joback Method
cpg	478.71	J/mol×K	522.42	Joback Method
cpg	498.28	J/mol×K	552.99	Joback Method
cpg	516.88	J/mol×K	583.57	Joback Method
cpg	534.57	J/mol×K	614.14	Joback Method
cpg	551.36	J/mol×K	644.71	Joback Method
cpg	567.31	J/mol×K	675.28	Joback Method
dvisc	0.1493107	Pa×s	178.69	Joback Method
dvisc	0.0130532	Pa×s	230.88	Joback Method

dvisc	0.0028030	Pa×s	283.08	Joback Method
dvisc	0.0009717	Pa×s	335.27	Joback Method
dvisc	0.0004481	Pa×s	387.46	Joback Method
dvisc	0.0002484	Pa×s	439.66	Joback Method
dvisc	0.0001560	Pa×s	491.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R306017&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
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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