

2,2,7,7-Tetramethyloctane

Inchi:	InChI=1S/C12H26/c1-11(2,3)9-7-8-10-12(4,5)6/h7-10H2,1-6H3
InchiKey:	QZUFNKONEPLWBC-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CC(C)(C)CCCC(C)(C)C
Mol. weight [g/mol]:	170.33
CAS:	1071-31-4

Physical Properties

Property code	Value	Unit	Source
gf	55.84	kJ/mol	Joback Method
hf	-308.51	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	39.71	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1013.00		NIST Webbook
rinpol	1036.75		NIST Webbook
rinpol	1036.70		NIST Webbook
rinpol	1035.93		NIST Webbook
rinpol	1039.50		NIST Webbook
rinpol	1039.44		NIST Webbook
rinpol	1038.54		NIST Webbook
rinpol	1036.70		NIST Webbook
rinpol	1013.00		NIST Webbook
tb	459.00 ± 3.00	K	NIST Webbook
tb	461.00 ± 8.00	K	NIST Webbook
tc	648.06	K	Joback Method
tf	319.00 ± 3.00	K	NIST Webbook
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.01	J/mol×K	467.50	Joback Method
cpg	430.55	J/mol×K	497.59	Joback Method
cpg	449.07	J/mol×K	527.69	Joback Method
cpg	466.62	J/mol×K	557.78	Joback Method
cpg	483.25	J/mol×K	587.87	Joback Method
cpg	498.99	J/mol×K	617.96	Joback Method
cpg	513.90	J/mol×K	648.06	Joback Method
dvisc	0.0149911	Paxs	229.84	Joback Method
dvisc	0.0043865	Paxs	269.45	Joback Method
dvisc	0.0017587	Paxs	309.06	Joback Method
dvisc	0.0008679	Paxs	348.67	Joback Method
dvisc	0.0004947	Paxs	388.28	Joback Method
dvisc	0.0003129	Paxs	427.89	Joback Method
dvisc	0.0002139	Paxs	467.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.35260e+01
Coeff. B	-3.26765e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	338.15
Temperature range (K), max.	489.10

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1071314&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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