

2,2,6,6-Tetramethylheptane

Inchi:	InChI=1S/C11H24/c1-10(2,3)8-7-9-11(4,5)6/h7-9H2,1-6H3
InchiKey:	GKNMBVVJQTDWDR-TUHFFFAOYSA-N
Formula:	C11H24
SMILES:	CC(C)(C)CCCC(C)(C)C
Mol. weight [g/mol]:	156.31
CAS:	40117-45-1

Physical Properties

Property code	Value	Unit	Source
gf	47.42	kJ/mol	Joback Method
hf	-287.87	kJ/mol	Joback Method
hfus	9.42	kJ/mol	Joback Method
hvap	37.49	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.249		Crippen Method
mvol	165.850	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
tb	444.62	K	Joback Method
tc	626.80	K	Joback Method
tf	218.57	K	Joback Method
vc	0.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.82	J/molxK	444.62	Joback Method
cpg	382.75	J/molxK	474.98	Joback Method
cpg	400.68	J/molxK	505.35	Joback Method
cpg	417.64	J/molxK	535.71	Joback Method
cpg	433.70	J/molxK	566.07	Joback Method
cpg	448.89	J/molxK	596.43	Joback Method
cpg	463.25	J/molxK	626.80	Joback Method
dvisc	0.0167899	Paxs	218.57	Joback Method
dvisc	0.0049116	Paxs	256.25	Joback Method

dvisc	0.0019690	Paxs	293.92	Joback Method
dvisc	0.0009716	Paxs	331.60	Joback Method
dvisc	0.0005538	Paxs	369.27	Joback Method
dvisc	0.0003502	Paxs	406.95	Joback Method
dvisc	0.0002394	Paxs	444.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34542e+01
Coeff. B	-3.09874e+03
Coeff. C	-8.54500e+01
Temperature range (K), min.	320.80
Temperature range (K), max.	466.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40117451&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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