3,3-Diethyloctane

Inchi: InChI=1S/C12H26/c1-5-9-10-11-12(6-2,7-3)8-4/h5-11H2,1-4H3
InchiKey: DGJISSKLLWWXTG-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCCCC(CC)(CC)CC
Mol. weight [g/mol]: 170.33
CAS: 17302-40-8

Physical Properties

Property code	Value	Unit	Source
gf	53.00	kJ/mol	Joback Method
hf	-299.76	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	41.01	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.783		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
tb	470.73	K	Joback Method
tc	640.99	K	Joback Method
tf	227.42	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.96	J/mol×K	470.73	Joback Method
cpg	491.58	J/mol×K	612.61	Joback Method
cpg	476.54	J/mol×K	584.24	Joback Method
cpg	460.79	J/mol×K	555.86	Joback Method
cpg	444.30	J/mol×K	527.48	Joback Method
cpg	427.03	J/mol×K	499.11	Joback Method
cpg	505.93	J/mol×K	640.99	Joback Method

dvisc	0.0002128	Pa×s	470.73	Joback Method
dvisc	0.0002979	Pa×s	430.18	Joback Method
dvisc	0.0004474	Pa×s	389.63	Joback Method
dvisc	0.0007385	Pa×s	349.07	Joback Method
dvisc	0.0013906	Pa×s	308.52	Joback Method
dvisc	0.0031716	Pa×s	267.97	Joback Method
dvisc	0.0097058	Pa×s	227.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39478e+01
Coeff. B	-3.60895e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	355.51
Temperature range (K), max.	509.20

Sources

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=R522848&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/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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