

Decane, 2,4,6-trimethyl-

Other names:	2,4,6-Trimethyldecane
Inchi:	InChI=1S/C13H28/c1-6-7-8-12(4)10-13(5)9-11(2)3/h11-13H,6-10H2,1-5H3
InchiKey:	NPHSALVLRUCAFH-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCCCC(C)CC(C)CC(C)C
Mol. weight [g/mol]:	184.36
CAS:	62108-27-4

Physical Properties

Property code	Value	Unit	Source
gf	51.26	kJ/mol	Joback Method
hf	-327.49	kJ/mol	Joback Method
hfus	18.86	kJ/mol	Joback Method
hvap	43.37	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.885		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	1121.00		NIST Webbook
tb	495.52	K	Joback Method
tc	665.29	K	Joback Method
tf	191.27	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.81	J/mol×K	495.52	Joback Method
cpg	474.51	J/mol×K	523.81	Joback Method
cpg	492.46	J/mol×K	552.11	Joback Method
cpg	509.67	J/mol×K	580.40	Joback Method
cpg	526.17	J/mol×K	608.70	Joback Method
cpg	541.98	J/mol×K	636.99	Joback Method
cpg	557.11	J/mol×K	665.29	Joback Method

dvisc	0.0334373	Pa×s	191.27	Joback Method
dvisc	0.0054966	Pa×s	241.98	Joback Method
dvisc	0.0016891	Pa×s	292.69	Joback Method
dvisc	0.0007355	Pa×s	343.39	Joback Method
dvisc	0.0003966	Pa×s	394.10	Joback Method
dvisc	0.0002462	Pa×s	444.81	Joback Method
dvisc	0.0001685	Pa×s	495.52	Joback Method
hvae	48.70	kJ/mol	415.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.69641e+01
Coeff. B	-5.93186e+03
Coeff. C	3.05700e+00
Temperature range (K), min.	352.64
Temperature range (K), max.	506.00

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108274&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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