

Decane, 2,3,7-trimethyl-

Other names:	2,3,7-Trimethyldecane
Inchi:	InChI=1S/C13H28/c1-6-8-12(4)9-7-10-13(5)11(2)3/h11-13H,6-10H2,1-5H3
InchiKey:	HTTBAQLJKLJCSR-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCCC(C)CCCC(C)C(C)C
Mol. weight [g/mol]:	184.36
CAS:	62238-13-5

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	1466.00		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/molxK	495.52	Joback Method
cpg	474.51	J/molxK	523.81	Joback Method
cpg	492.46	J/molxK	552.11	Joback Method
cpg	509.67	J/molxK	580.40	Joback Method
cpg	526.17	J/molxK	608.70	Joback Method
cpg	541.98	J/molxK	636.99	Joback Method
cpg	557.11	J/molxK	665.29	Joback Method

dvisc	0.0334373	Paxs	191.27	Joback Method
dvisc	0.0054966	Paxs	241.98	Joback Method
dvisc	0.0016891	Paxs	292.69	Joback Method
dvisc	0.0007355	Paxs	343.39	Joback Method
dvisc	0.0003966	Paxs	394.10	Joback Method
dvisc	0.0002462	Paxs	444.81	Joback Method
dvisc	0.0001685	Paxs	495.52	Joback Method

Sources

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=C62238135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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