

Heptane, 5-ethyl-2,2,3-trimethyl-

Inchi:	InChI=1S/C12H26/c1-7-11(8-2)9-10(3)12(4,5)6/h10-11H,7-9H2,1-6H3
InchiKey:	OOIGDPTZPWRGHN-UHFFFAOYSA-N
Formula:	C12H26
SMILES:	CCC(CC)CC(C)C(C)(C)C
Mol. weight [g/mol]:	170.33
CAS:	62199-06-8

Physical Properties

Property code	Value	Unit	Source
gf	48.12	kJ/mol	Joback Method
hf	-310.32	kJ/mol	Joback Method
hfus	12.38	kJ/mol	Joback Method
hvap	40.23	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.495		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
tb	469.85	K	Joback Method
tc	647.37	K	Joback Method
tf	197.42	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.07	J/molxK	469.85	Joback Method
cpg	428.06	J/molxK	499.44	Joback Method
cpg	446.17	J/molxK	529.02	Joback Method
cpg	463.43	J/molxK	558.61	Joback Method
cpg	479.87	J/molxK	588.20	Joback Method
cpg	495.52	J/molxK	617.78	Joback Method
cpg	510.41	J/molxK	647.37	Joback Method
dvisc	0.0334827	Paxs	197.42	Joback Method
dvisc	0.0063428	Paxs	242.83	Joback Method

dvisc	0.0020295	Paxs	288.23	Joback Method
dvisc	0.0008855	Paxs	333.63	Joback Method
dvisc	0.0004713	Paxs	379.04	Joback Method
dvisc	0.0002871	Paxs	424.45	Joback Method
dvisc	0.0001924	Paxs	469.85	Joback Method

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=C62199068&Units=SI

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

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