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/mol×K	469.85	Joback Method
cpg	495.52	J/mol×K	617.78	Joback Method
cpg	479.87	J/mol×K	588.20	Joback Method
cpg	463.43	J/mol×K	558.61	Joback Method
cpg	446.17	J/mol×K	529.02	Joback Method
cpg	428.06	J/mol×K	499.44	Joback Method
cpg	510.41	J/mol×K	647.37	Joback Method
dvisc	0.0001924	Pa×s	469.85	Joback Method
dvisc	0.0002871	Pa×s	424.45	Joback Method

dvisc	0.0004713	Pa×s	379.04	Joback Method
dvisc	0.0008855	Pa×s	333.63	Joback Method
dvisc	0.0020295	Pa×s	288.23	Joback Method
dvisc	0.0063428	Pa×s	242.83	Joback Method
dvisc	0.0334827	Pa×s	197.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62199068&Units=SI
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

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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