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]: 170.34

Physical Properties

Property code	Value	Unit	Source
af	0.4074		Cheméo Relay (1.0)
gf	48.12	kJ/mol	Joback Method
hf	-299.79	kJ/mol	Cheméo Relay (1.0)
hfus	12.38	kJ/mol	Joback Method
hvap	50.73	kJ/mol	Cheméo Relay (1.0)
logp	4.495		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
tb	464.86	K	Cheméo Relay (1.0)
tc	629.36	K	Cheméo Relay (1.0)
tf	180.79	K	Cheméo Relay (1.0)
vc	0.632	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.07	J/mol×K	469.85	Joback Method
cpg	428.06	J/mol×K	499.44	Joback Method
cpg	446.17	J/mol×K	529.02	Joback Method
cpg	463.43	J/mol×K	558.61	Joback Method
cpg	479.87	J/mol×K	588.20	Joback Method
cpg	495.52	J/mol×K	617.78	Joback Method
cpg	510.41	J/mol×K	647.37	Joback Method
dvisc	0.0334827	Pa×s	197.42	Joback Method
dvisc	0.0063428	Pa×s	242.83	Joback Method
dvisc	0.0020295	Pa×s	288.23	Joback Method

dvisc	0.0008855	Pa×s	333.63	Joback Method
dvisc	0.0004713	Pa×s	379.04	Joback Method
dvisc	0.0002871	Pa×s	424.45	Joback Method
dvisc	0.0001924	Pa×s	469.85	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62199068&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
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