3,4-Dimethylheptane, threo

Other names:	«beta»-3,4-dimethylheptane
	Heptane, 3,4-dimethyl-, threo-
	3,4-Dimethylheptane, (L)
Inchi:	InChI=1S/C9H20/c1-5-7-9(4)8(3)6-2/h8-9H,5-7H2,1-4H3/t8-,9-/m1/s1
InchiKey:	MAKRYGRRIKSDES-RKDXNWHRSA-N
Formula:	C9H20
SMILES:	CCCC(C)C(C)CC
Mol. weight [g/mol]:	128.26

Physical Properties

Property code	Value	Unit	Source
gf	20.02	kJ/mol	Joback Method
hf	-239.65	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	34.85	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.469		Crippen Method
mcvol	137.670	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	862.60		NIST Webbook
rinpol	855.70		NIST Webbook
rinpol	856.40		NIST Webbook
rinpol	857.90		NIST Webbook
rinpol	857.90		NIST Webbook
rinpol	859.80		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	849.20		NIST Webbook
tb	404.44	K	Joback Method
tc	574.89	K	Joback Method
tf	161.19	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.52	J/mol×K	404.44	Joback Method
cpg	287.44	J/mol×K	432.85	Joback Method
cpg	301.80	J/mol×K	461.26	Joback Method
cpg	315.61	J/mol×K	489.67	Joback Method
cpg	328.88	J/mol×K	518.07	Joback Method
cpg	341.62	J/mol×K	546.48	Joback Method
cpg	353.86	J/mol×K	574.89	Joback Method
dvisc	0.0224972	Pa×s	161.19	Joback Method
dvisc	0.0048330	Pa×s	201.73	Joback Method
dvisc	0.0017372	Pa×s	242.27	Joback Method
dvisc	0.0008373	Pa×s	282.81	Joback Method
dvisc	0.0004846	Pa×s	323.36	Joback Method
dvisc	0.0003168	Pa×s	363.90	Joback Method
dvisc	0.0002255	Pa×s	404.44	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R251962&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

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