

3,5-Dimethylheptane, erythro

Other names:	Heptane, 3,5-dimethyl-, meso
Inchi:	InChI=1S/C9H20/c1-5-8(3)7-9(4)6-2/h8-9H,5-7H2,1-4H3/t8-,9+
InchiKey:	DZJTZGHZAWTWGA-DTORHVGOSA-N
Formula:	C9H20
SMILES:	CCC(C)CC(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	834.10		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	833.70		NIST Webbook
rinpol	833.50		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/molxK	404.44	Joback Method
cpg	341.62	J/molxK	546.48	Joback Method
cpg	328.88	J/molxK	518.07	Joback Method
cpg	315.61	J/molxK	489.67	Joback Method
cpg	301.80	J/molxK	461.26	Joback Method

cpg	287.44	J/molxK	432.85	Joback Method
cpg	353.86	J/molxK	574.89	Joback Method
dvisc	0.0002255	Paxs	404.44	Joback Method
dvisc	0.0003168	Paxs	363.90	Joback Method
dvisc	0.0004846	Paxs	323.36	Joback Method
dvisc	0.0008373	Paxs	282.81	Joback Method
dvisc	0.0017372	Paxs	242.27	Joback Method
dvisc	0.0048330	Paxs	201.73	Joback Method
dvisc	0.0224972	Paxs	161.19	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=R293535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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