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	834.00		NIST Webbook
rinpol	833.70		NIST Webbook
rinpol	833.50		NIST Webbook
rinpol	834.10		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	341.62	J/mol×K	546.48	Joback Method
cpg	328.88	J/mol×K	518.07	Joback Method
cpg	315.61	J/mol×K	489.67	Joback Method
cpg	301.80	J/mol×K	461.26	Joback Method

cpg	287.44	J/mol×K	432.85	Joback Method
cpg	353.86	J/mol×K	574.89	Joback Method
dvisc	0.0002255	Pa×s	404.44	Joback Method
dvisc	0.0003168	Pa×s	363.90	Joback Method
dvisc	0.0004846	Pa×s	323.36	Joback Method
dvisc	0.0008373	Pa×s	282.81	Joback Method
dvisc	0.0017372	Pa×s	242.27	Joback Method
dvisc	0.0048330	Pa×s	201.73	Joback Method
dvisc	0.0224972	Pa×s	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