2,2-Dimethyl-3-heptene trans

Other names: trans-2,2-Dimethyl-3-heptene
3-Heptene, 2,2-dimethyl-, (E)-
(E)-2,2-dimethylhept-3-ene
Inchi: InChI=1S/C9H18/c1-5-6-7-8-9(2,3)4/h7-8H,5-6H2,1-4H3/b8-7+
InchiKey: BQOCYCICSYUPRF-BQYQJAHWSA-N
Formula: C9H18
SMILES: CCCC=CC(C)(C)C
Mol. weight [g/mol]: 126.24
CAS: 19550-75-5

Physical Properties

Property code	Value	Unit	Source
gf	107.96	kJ/mol	Joback Method
hf	-120.62	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	34.29	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.389		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	802.00		NIST Webbook
tb	406.25	K	Joback Method
tc	588.59	K	Joback Method
tf	188.53	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.57	J/mol×K	406.25	Joback Method
cpg	329.51	J/mol×K	558.20	Joback Method
cpg	317.00	J/mol×K	527.81	Joback Method
cpg	303.79	J/mol×K	497.42	Joback Method
cpg	289.84	J/mol×K	467.03	Joback Method

cpg	275.11	J/mol×K	436.64	Joback Method
cpg	341.36	J/mol×K	588.59	Joback Method
dvisc	0.0002180	Pa×s	406.25	Joback Method
dvisc	0.0003038	Pa×s	369.96	Joback Method
dvisc	0.0004551	Pa×s	333.68	Joback Method
dvisc	0.0007523	Pa×s	297.39	Joback Method
dvisc	0.0014301	Pa×s	261.10	Joback Method
dvisc	0.0033453	Pa×s	224.82	Joback Method
dvisc	0.0108529	Pa×s	188.53	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=C19550755&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