Heptane, 2,3,5-trimethyl-

Other names: 2,3,5-Trimethylheptane
Inchi: InChI=1S/C10H22/c1-6-9(4)7-10(5)8(2)3/h8-10H,6-7H2,1-5H3
InchiKey: YKPNYFKOKKKGNM-UHFFFAOYSA-N
Formula: C10H22
SMILES: CCC(C)CC(C)C(C)C
Mol. weight [g/mol]: 142.28
CAS: 20278-85-7

Physical Properties

Property code	Value	Unit	Source
gf	26.00	kJ/mol	Joback Method
hf	-265.57	kJ/mol	Joback Method
hfus	11.09	kJ/mol	Joback Method
hvap	47.30	kJ/mol	NIST Webbook
log10ws	-3.28		Crippen Method
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	913.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	912.90		NIST Webbook
tb	426.88	K	Joback Method
tc	600.24	K	Joback Method
tf	157.46	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.23	J/mol×K	426.88	Joback Method

cpg	331.59	J/mol×K	455.77	Joback Method
cpg	347.31	J/mol×K	484.67	Joback Method
cpg	362.39	J/mol×K	513.56	Joback Method
cpg	376.87	J/mol×K	542.45	Joback Method
cpg	390.75	J/mol×K	571.35	Joback Method
cpg	404.05	J/mol×K	600.24	Joback Method
dvisc	0.0495825	Pa×s	157.46	Joback Method
dvisc	0.0072381	Pa×s	202.36	Joback Method
dvisc	0.0021254	Pa×s	247.27	Joback Method
dvisc	0.0009096	Pa×s	292.17	Joback Method
dvisc	0.0004880	Pa×s	337.07	Joback Method
dvisc	0.0003031	Pa×s	381.98	Joback Method
dvisc	0.0002081	Pa×s	426.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42428e+01
Coeff. B	-3.63248e+03
Coeff. C	-5.64370e+01
Temperature range (K), min.	316.73
Temperature range (K), max.	463.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.96834e+01
Coeff. B	-8.91054e+03
Coeff. C	-1.25077e+01
Coeff. D	7.59600e-06
Temperature range (K), min.	317.15
Temperature range (K), max.	612.80

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=132
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20278857&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=132
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume