2,3-Dimethyl-1-hexene

Other names: 1-Hexene, 2,3-dimethyl-
2,3-Dimethylhex-1-ene
Inchi: InChI=1S/C8H16/c1-5-6-8(4)7(2)3/h8H,2,5-6H2,1,3-4H3
InchiKey: LVLXQRZPKUFJJQ-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(C)C(C)CCC
Mol. weight [g/mol]: 112.21
CAS: 16746-86-4

Physical Properties

Property code	Value	Unit	Source
gf	93.33	kJ/mol	Joback Method
hf	-98.09	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	38.50	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	748.80		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	746.70		NIST Webbook
rinpol	737.50		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	748.80		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	739.10		NIST Webbook
rinpol	740.60		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	741.00		NIST Webbook

rinpol	741.00		NIST Webbook
rinpol	739.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	746.70		NIST Webbook
tb	383.69 ± 0.20	K	NIST Webbook
tb	383.69 ± 0.40	K	NIST Webbook
tb	383.69 ± 0.60	K	NIST Webbook
tc	552.61	K	Joback Method
tf	149.20	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.59	J/mol×K	378.56	Joback Method
cpg	230.69	J/mol×K	407.57	Joback Method
cpg	243.26	J/mol×K	436.58	Joback Method
cpg	255.31	J/mol×K	465.59	Joback Method
cpg	266.87	J/mol×K	494.59	Joback Method
cpg	277.94	J/mol×K	523.60	Joback Method
cpg	288.55	J/mol×K	552.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31705e+01
Coeff. B	-2.88169e+03
Coeff. C	-5.64010e+01
Temperature range (K), min.	280.08
Temperature range (K), max.	423.07

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16746864&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=283
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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