2-Methyl-1,4-pentadiene

Other names: 2-METHYL-4-PENTADIENE
2-methylpenta-1,4-diene
Inchi: InChI=1S/C6H10/c1-4-5-6(2)3/h4H,1-2,5H2,3H3
InchiKey: DRWYRROCDFQZQF-UHFFFAOYSA-N
Formula: C6H10
SMILES: C=CCC(=C)C
Mol. weight [g/mol]: 82.15
CAS: 763-30-4

Physical Properties

Property code	Value	Unit	Source
hf	78.15	kJ/mol	Cheméo Relay (1.0)
hfus	7.43	kJ/mol	Joback Method
hvap	28.75	kJ/mol	Cheméo Relay (1.0)
ie	9.07	eV	Cheméo Relay (1.0)
log10ws	-2.72		Cheméo Relay (1.0)
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	559.00		NIST Webbook
tb	328.47	K	Cheméo Relay (1.0)
tc	501.07	K	Cheméo Relay (1.0)
tf	141.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.15	J/mol×K	329.92	Joback Method
cpg	142.61	J/mol×K	358.89	Joback Method
cpg	151.66	J/mol×K	387.85	Joback Method
cpg	160.31	J/mol×K	416.82	Joback Method
cpg	168.57	J/mol×K	445.79	Joback Method
cpg	176.46	J/mol×K	474.76	Joback Method
cpg	184.00	J/mol×K	503.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33360e+01
Coeff. B	-2.48932e+03
Coeff. C	-4.36500e+01
Temperature range (K), min.	234.43
Temperature range (K), max.	353.87

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C763304&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol383.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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