Hexane, 2-methyl-4-methylene-

Other names: 1-Pentene, 2-ethyl-4-methyl
2-Ethyl-4-methyl-1-pentene
2-Ethyl-4-methylpent-1-ene
Inchi: InChI=1S/C8H16/c1-5-8(4)6-7(2)3/h7H,4-6H2,1-3H3
InchiKey: TVBQWTDYXVGWJL-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=C(CC)CC(C)C
Mol. weight [g/mol]: 112.21
CAS: 3404-80-6

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	745.70		NIST Webbook
rinpol	731.20		NIST Webbook
rinpol	737.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	745.70		NIST Webbook
tb	378.56	K	Joback Method
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

Sources

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/files/research/kdb/mol/mol323.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404806&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume