2-Methyl-3-ethyl-2-heptene

Other names: C4H9C(C2H5)=C(CH3)2
3-Ethyl-2-methyl-2-heptene
Inchi: InChI=1S/C10H20/c1-5-7-8-10(6-2)9(3)4/h5-8H2,1-4H3
InchiKey: JCVDGJIYXBDDCK-UHFFFAOYSA-N
Formula: C10H20
SMILES: CCCCC(CC)=C(C)C
Mol. weight [g/mol]: 140.27
CAS: 19780-61-1

Physical Properties

Property code	Value	Unit	Source
gf	96.44	kJ/mol	Joback Method
hf	-152.09	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	37.97	kJ/mol	Joback Method
ie	8.10 ± 0.01	eV	NIST Webbook
log10ws	-3.86		Crippen Method
logp	3.923		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1073.00		NIST Webbook
rinpol	979.10		NIST Webbook
rinpol	1073.00		NIST Webbook
tb	432.12	K	Joback Method
tc	608.78	K	Joback Method
tf	169.46	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.15	J/mol×K	432.12	Joback Method
cpg	315.61	J/mol×K	461.56	Joback Method
cpg	330.39	J/mol×K	491.01	Joback Method

cpg	344.52	J/mol×K	520.45	Joback Method
cpg	358.03	J/mol×K	549.89	Joback Method
cpg	370.94	J/mol×K	579.34	Joback Method
cpg	383.26	J/mol×K	608.78	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=C19780611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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