3-Heptyne, 2-methyl

Inchi: InChI=1S/C8H14/c1-4-5-6-7-8(2)3/h8H,4-5H2,1-3H3
InchiKey: HLWVADIAYHXLDP-UHFFFAOYSA-N
Formula: C8H14
SMILES: CCCC#CC(C)C
Mol. weight [g/mol]: 110.20

Physical Properties

Property code	Value	Unit	Source
gf	216.84	kJ/mol	Joback Method
hf	58.57	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	35.17	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.446		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	753.00		NIST Webbook
rinpol	753.00		NIST Webbook
tb	391.00	K	Joback Method
tc	582.81	K	Joback Method
tf	271.02	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.33	J/mol×K	391.00	Joback Method
cpg	220.75	J/mol×K	422.97	Joback Method
cpg	232.68	J/mol×K	454.94	Joback Method
cpg	244.12	J/mol×K	486.91	Joback Method
cpg	255.09	J/mol×K	518.88	Joback Method
cpg	265.59	J/mol×K	550.85	Joback Method
cpg	275.65	J/mol×K	582.81	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=R66643&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
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