4,5-Nonadiene

Inchi: InChI=1S/C9H16/c1-3-5-7-9-8-6-4-2/h7-8H,3-6H2,1-2H3
InchiKey: NYLHDUHTALIPLY-UHFFFAOYSA-N
Formula: C9H16
SMILES: CCCC=C=CCCC
Mol. weight [g/mol]: 124.22
CAS: 821-74-9

Physical Properties

Property code	Value	Unit	Source
gf	233.40	kJ/mol	Joback Method
hf	50.91	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	36.02	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.298		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	412.75	K	Joback Method
tc	594.66	K	Joback Method
tf	192.62	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.93	J/mol×K	412.75	Joback Method
cpg	261.13	J/mol×K	443.07	Joback Method
cpg	273.80	J/mol×K	473.39	Joback Method
cpg	285.96	J/mol×K	503.70	Joback Method
cpg	297.63	J/mol×K	534.02	Joback Method
cpg	308.80	J/mol×K	564.34	Joback Method
cpg	319.51	J/mol×K	594.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821749&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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