3,4-Heptadiene

Other names: 1,3-Diethylallene
Inchi: InChI=1S/C7H12/c1-3-5-7-6-4-2/h5-6H,3-4H2,1-2H3
InchiKey: ZLYMNRDOPVPQPY-UHFFFAOYSA-N
Formula: C7H12
SMILES: CCC=C=CCC
Mol. weight [g/mol]: 96.17
CAS: 2454-31-1

Physical Properties

Property code	Value	Unit	Source
gf	216.56	kJ/mol	Joback Method
hf	92.19	kJ/mol	Joback Method
hfus	16.22	kJ/mol	Joback Method
hvap	31.57	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.518		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	366.99	K	Joback Method
tc	550.88	K	Joback Method
tf	170.08	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.54	J/mol×K	366.99	Joback Method
cpg	183.12	J/mol×K	397.64	Joback Method
cpg	193.29	J/mol×K	428.29	Joback Method
cpg	203.06	J/mol×K	458.94	Joback Method
cpg	212.44	J/mol×K	489.59	Joback Method
cpg	221.45	J/mol×K	520.23	Joback Method
cpg	230.09	J/mol×K	550.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2454311&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