

(S)-3-methylheptane

Inchi:	InChI=1S/C8H18/c1-4-6-7-8(3)5-2/h8H,4-7H2,1-3H3/t8-/m1/s1
InchiKey:	LAIUFBWHERIJH-MRVPVSSYSA-N
Formula:	C8H18
SMILES:	CCCCC(C)CC
Mol. weight [g/mol]:	114.23
CAS:	6131-25-5

Physical Properties

Property code	Value	Unit	Source
gf	14.04	kJ/mol	Joback Method
hf	-213.73	kJ/mol	Joback Method
hfus	12.95	kJ/mol	Joback Method
hvap	33.01	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	3.223		Crippen Method
mcvol	123.580	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	390.15 ± 2.00	K	NIST Webbook
tc	549.20	K	Joback Method
tf	164.92	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.14	J/mol×K	382.00	Joback Method
cpg	294.38	J/mol×K	521.33	Joback Method
cpg	282.86	J/mol×K	493.46	Joback Method
cpg	270.88	J/mol×K	465.60	Joback Method
cpg	258.44	J/mol×K	437.73	Joback Method
cpg	245.53	J/mol×K	409.87	Joback Method
cpg	305.46	J/mol×K	549.20	Joback Method
dvisc	0.0002373	Paxs	382.00	Joback Method
dvisc	0.0003209	Paxs	345.82	Joback Method

dvisc	0.0004656	Paxs	309.64	Joback Method
dvisc	0.0007454	Paxs	273.46	Joback Method
dvisc	0.0013776	Paxs	237.28	Joback Method
dvisc	0.0031758	Paxs	201.10	Joback Method
dvisc	0.0105616	Paxs	164.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6131255&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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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