6-Methylheptanal

Other names: Heptanal, 6-methyl-
Inchi: InChI=1S/C8H16O/c1-8(2)6-4-3-5-7-9/h7-8H,3-6H2,1-2H3
InchiKey: LCEHKIHBHIJPCD-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CC(C)CCCCC=O
Mol. weight [g/mol]: 128.21
CAS: 63885-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-85.48	kJ/mol	Joback Method
hf	-299.31	kJ/mol	Joback Method
hfus	15.24	kJ/mol	Joback Method
hvap	39.73	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	948.00		NIST Webbook
tb	430.66	K	Joback Method
tc	605.22	K	Joback Method
tf	206.92	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.75	J/mol×K	430.66	Joback Method
cpg	269.26	J/mol×K	459.75	Joback Method
cpg	281.26	J/mol×K	488.85	Joback Method
cpg	292.77	J/mol×K	517.94	Joback Method
cpg	303.81	J/mol×K	547.04	Joback Method
cpg	314.39	J/mol×K	576.13	Joback Method
cpg	324.51	J/mol×K	605.22	Joback Method

dvisc	0.0077983	Pa×s	206.92	Joback Method
dvisc	0.0030008	Pa×s	244.21	Joback Method
dvisc	0.0014872	Pa×s	281.50	Joback Method
dvisc	0.0008686	Pa×s	318.79	Joback Method
dvisc	0.0005678	Pa×s	356.08	Joback Method
dvisc	0.0004023	Pa×s	393.37	Joback Method
dvisc	0.0003026	Pa×s	430.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63885096&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume