

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)CCCC=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/molxK	430.66	Joback Method
cpg	269.26	J/molxK	459.75	Joback Method
cpg	281.26	J/molxK	488.85	Joback Method
cpg	292.77	J/molxK	517.94	Joback Method
cpg	303.81	J/molxK	547.04	Joback Method
cpg	314.39	J/molxK	576.13	Joback Method
cpg	324.51	J/molxK	605.22	Joback Method

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

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63885096&Units=SI

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

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