

(E)-6-Methylhept-4-en-1-ol

Inchi:	InChI=1S/C8H16O/c1-8(2)6-4-3-5-7-9/h4,6,8-9H,3,5,7H2,1-2H3/b6-4+
InchiKey:	FRDGUFZXMNVORS-GQCTYLIASA-N
Formula:	C8H16O
SMILES:	CC(C)C=CCCCO
Mol. weight [g/mol]:	128.21
CAS:	855901-81-4

Physical Properties

Property code	Value	Unit	Source
gf	-42.56	kJ/mol	Joback Method
hf	-248.74	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	49.65	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.971		Crippen Method
mvol	125.150	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1020.10		NIST Webbook
rinpol	1020.10		NIST Webbook
tb	478.34	K	Joback Method
tc	648.44	K	Joback Method
tf	220.66	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.48	J/mol×K	478.34	Joback Method
cpg	284.97	J/mol×K	506.69	Joback Method
cpg	295.95	J/mol×K	535.04	Joback Method
cpg	306.45	J/mol×K	563.39	Joback Method
cpg	316.47	J/mol×K	591.74	Joback Method
cpg	326.05	J/mol×K	620.09	Joback Method
cpg	335.20	J/mol×K	648.44	Joback Method

dvisc	0.1274533	Paxs	220.66	Joback Method
dvisc	0.0161573	Paxs	263.61	Joback Method
dvisc	0.0036535	Paxs	306.55	Joback Method
dvisc	0.0011905	Paxs	349.50	Joback Method
dvisc	0.0004958	Paxs	392.45	Joback Method
dvisc	0.0002455	Paxs	435.39	Joback Method
dvisc	0.0001379	Paxs	478.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C855901814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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