(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
mcvol	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	m3/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	Pa×s	220.66	Joback Method
dvisc	0.0161573	Pa×s	263.61	Joback Method
dvisc	0.0036535	Pa×s	306.55	Joback Method
dvisc	0.0011905	Pa×s	349.50	Joback Method
dvisc	0.0004958	Pa×s	392.45	Joback Method
dvisc	0.0002455	Pa×s	435.39	Joback Method
dvisc	0.0001379	Pa×s	478.34	Joback Method

Sources

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=C855901814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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